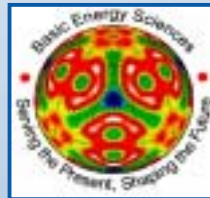


# Basic Energy Sciences at NREL

## Funded by the DOE Office of Science and DOE Office of Energy Efficiency and Renewable Energy



U.S. Department of Energy  
**Energy Efficiency  
and Renewable Energy**  
Bringing you a prosperous future where energy is  
clean, abundant, reliable, and affordable

**Satyen K. Deb**  
Director, Basic Sciences Center  
National Renewable Energy Laboratory  
Golden, CO 80401

# National Renewable Energy Laboratory

- Only national laboratory ***dedicated*** to renewable energy and energy efficiency R&D
- Research spans fundamental ***science*** to ***technology*** solutions
- ***Collaboration*** with industry and university partners is a hallmark
- Research programs ***linked*** to market opportunities



# Major NREL Technology Thrusts

## Supply Side

Wind Energy

Solar Photovoltaics

Concentrating Solar Power

Solar Buildings

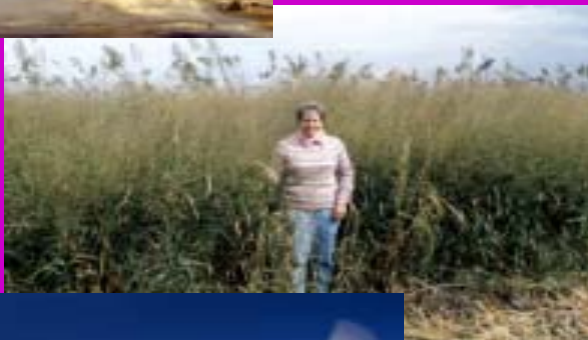
Biomass Power

Biofuels

Geothermal Energy

Hydrogen

Superconductivity



## Demand Side

Hybrid Vehicles

Fuels Utilization

Buildings Energy Technology

Federal Energy Management

Advanced Industrial Technologies

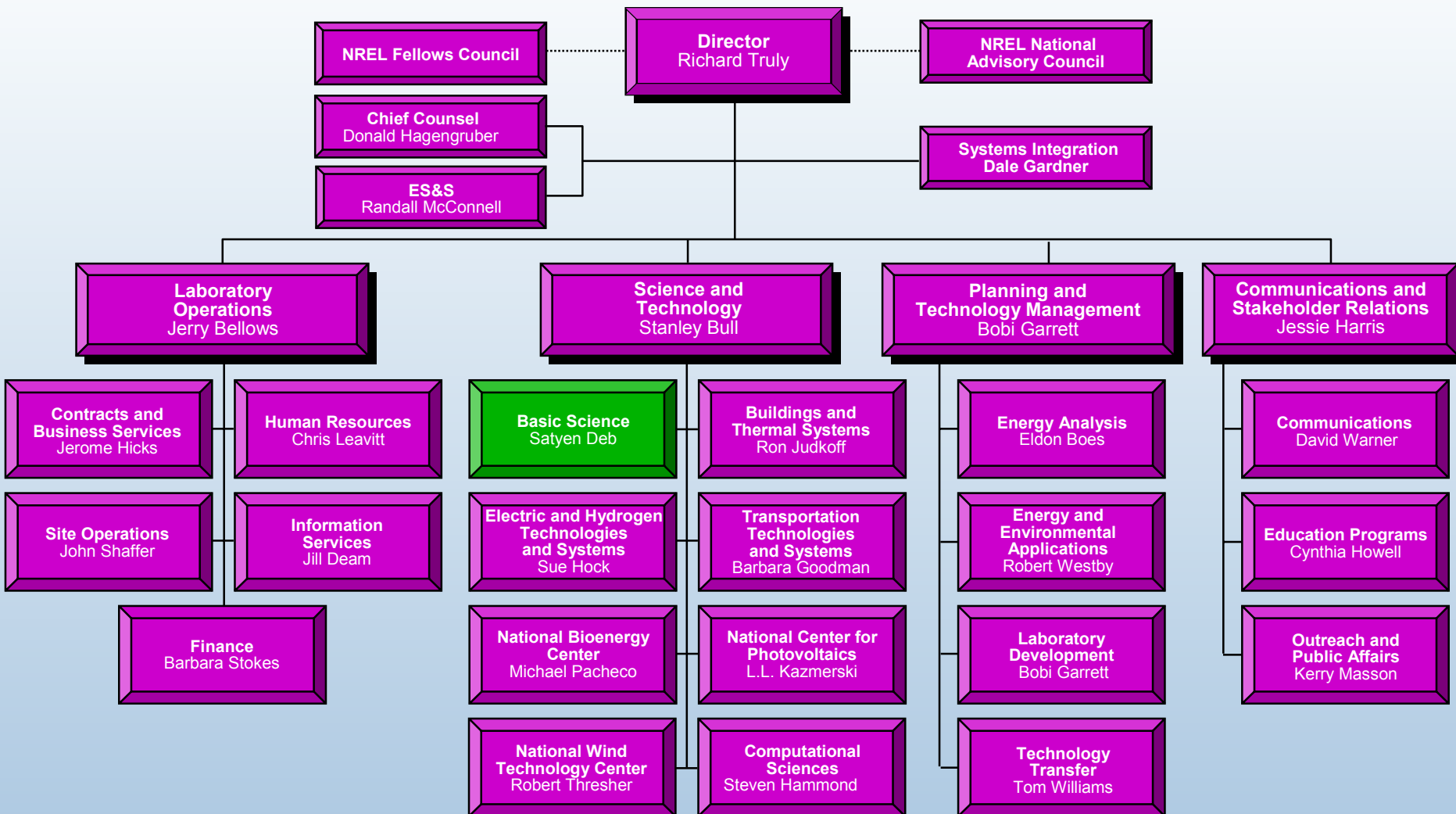
## Cross Cutting

Basic Energy Science

Analytical Studies

International Programs

# NREL Organization



# Center for Basic Sciences

## March 2004

**Satyen Deb, Director**

**Research Fellows: Nozik, Seibert, Zunger**

**Melody Mountz, Admin. Asst.**

**Group Manager  
Satyen Deb, Acting  
Materials Science**

**Consuelo Montano  
Admin. Asst.**

**Group Manager  
Garry Rumbles  
Chemical & Biosciences**

**Inger Jafari & Lynn Westdal  
Admin. Assts.**

### **Solid State Spectroscopy – Angelo Mascarenhas**

Brian Fluegel Steve Smith  
Yong Zhang Sebastian Francoeur (TOA)  
Seokhyun Yoon (PD)

### **Solid State Theory – Alex Zunger**

Sergey Barabash (PD) Gabriel Bester (PD)  
Volker Blum (PD) Marco Califano (NT)  
Sergey Dudiy (PD) Lixin He (PD)  
Stefan Lany (PD) Clas Persson (PD)  
Yu-Jun Zhao (PD) Joonhee An (PD)

### **Computational Materials Science – Su-Huai Wei**

Shengbai Zhang Iskander Batyrev (NT-RA)  
Pierre Carrier (PD) Gustavo Dalpian (PD)  
Yong-Hyun Kim (PD) David Segev (PD)  
Yufeng Zhao (PD) Mao-Hua Du (PD)

### **Optoelectronics – Roland Pitts**

Se-Hee Lee Edwin Tracy  
Ping Liu R. Davis Smith (PD)

### **Superconductivity – Raghu Bhattacharya**

Tapas Chaudhuri (TOA) Priscilla Spagnol (PD)

### **Chemical Science & Nanoscience – Arthur Nozik**

Randy Ellingson Sue Ferrere  
Arthur Frank Brian Gregg  
Mark Hanna Olga Micic  
Donald Selmarten Matthew Beard (PD)  
Si-Guang Chen (PD) Russ Cormier (C)  
Sophie Gledhill (PD) Marcus Jones (PD)  
Nikos Kopidakis (PD) Jim Murphy (TOA)  
Nathan Neale (PD) Jovan Nedeljkovic (SAB)  
Yong-su Park (PD) Jao van de Lagemaat (NT)  
Kyung-Byung Yoon (SAB) Pingrong Yu (TOA)  
Peng Zhang (PD)

### **Catalysis – Dan DuBois**

Calvin Curtis Alex Miedaner  
Rachel Newell (UG)

### **Energy Biosciences – Michael Seibert**

Maria Ghirardi Willard Hibbs  
Pin-Ching Maness Sharon Smolinski  
Dianne Ahmann (S) Rohit Datar (PD)  
Sasha Fedorov (PD) Paul King (PD)  
Lauren Nagy (G) Scott Plummer (G)  
Matthew Posewitz (NT-RA) Gary Vanzin (PD)  
Vekalet Tek (RA)

**Carbon-Based H<sub>2</sub> Storage  
Michael Heben  
Sr. Project Leader**

**Project  
Coordination  
External to NREL**

**Synthesis & Processing  
Sr. Research Scientist**

**Characterization of  
H<sub>2</sub> Storage  
Sr. Research Scientist**

**Theory/Modelling  
Sr. Research Scientist**

**Office of Science  
Nanoscience  
C-nanotube**

**Total Staff  
17.5 FTEs  
(7 Reg Staff, 6 PDs, 4Gs)  
Total Funding ~\$2.5M**

#### **Legend for Temporary Staff**

C = Consultant  
CR = CRADA  
G = Grad Student  
LW = Leased Worker  
NT = NREL Temp  
PD = Postdoc  
RA = Research Associate  
S = Student  
SRA = Sr. Research Associate  
SAB = Sabbatical  
TOA = Task Order Agreement  
UG = Undergrad Student

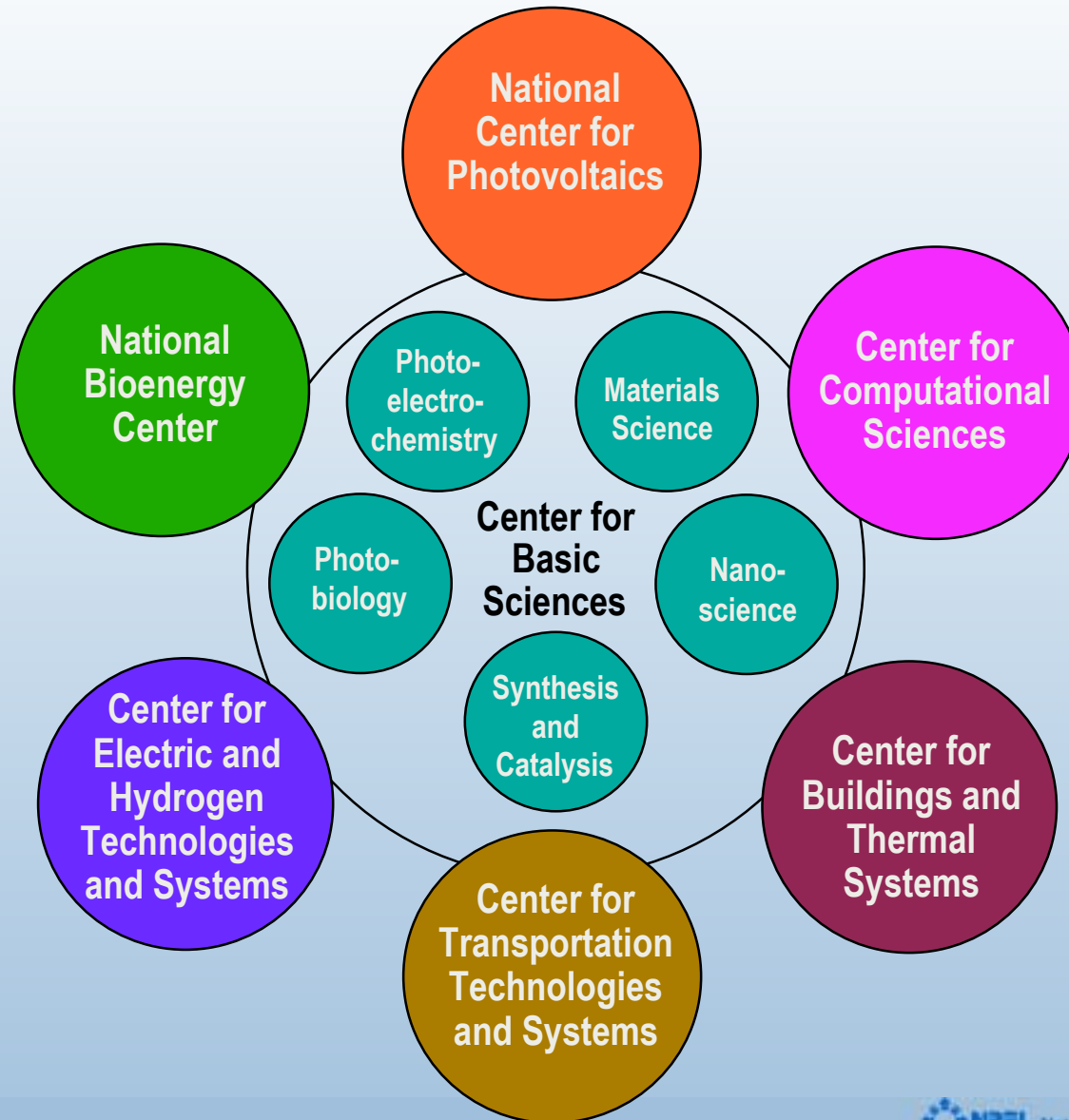
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# Mission Statement

## Basic Energy Science at NREL

NREL's Center for Basic Sciences performs fundamental research for DOE's Office of Science and Office of Energy Efficiency and Renewable Energy. Our mission is to provide fundamental knowledge in the basic sciences and engineering that will underpin new and improved renewable energy technologies. In support of this mission, NREL executes research in three areas— materials sciences, chemical sciences, and energy biosciences. NREL also integrates its fundamental research with applied R&D in several projects.

# Center for Basic Sciences Interactions



**Center for Basic Science  
Activities**  
Satyen Deb, Director

**By Science**

**Materials Science**

- Materials growth
- Thin films
- Nanostructures/  
superlattices/  
quantum dots
- Characterization  
(structural, optical  
and electrical)
- Solid state  
spectroscopy
- Condensed matter  
theory
- High  $T_c$  superconductors
- Electrochromics

**Bio Science**

- Photobiology
- Artificial  
photosynthesis
- Photosynthetic  
bacteria
- Biochemical  
processes
- Hydrogenase  
enzymes
- Chemometric  
methods

**Chemical Science**

- Photoelectrochemistry
- Interfacial photochemistry
- Molecular semiconductors
- Synthesis and catalysis
- Photoelectrolysis
- $H_2$  generation and storage
- Advanced batteries
- Nanoscale chemistry
- Colloidal semiconductor  
quantum dots

**By Technology**

- Photovoltaics (solar cells)
- Semiconductors and other  
optoelectronic devices
- Fuel production
- Hydrogen storage and sensors
- Chemical production
- “Smart” windows
- Fuel cells
- Batteries
- Superconductor
- Solid state LEDs
- $CO_2$  mitigation
- Bioremediation
- Nanoscale devices



# Material Sciences

## Goal

The goal of the Materials Sciences projects is to study the structural, optical, electrical, and defect properties of some exciting, new semiconductors and related materials for photovoltaics and other energy-related applications by using the state-of-the-art theoretical and experimental techniques.

## Approaches

- Ordering in III-V semiconductor alloy materials
- Physics of isoelectronic co-doping
- Doping bottlenecks in semiconductors
- Carbon nanotubes membranes
- Solid state theory and computational science
- Nanostructure materials
- Novel semiconductor and optoelectronic materials
- High  $T_C$  superconducting materials

# Photovoltaic Cells

## I. 1<sup>st</sup> Generation

- Single crystal Si
- Poly-grain Si

## II. 2<sup>nd</sup> Generation (Polycrystalline Thin Film)

- Amorphous Si
- Thin film Si
- $\text{CuInSe}_2$
- CdTe
- Dye-sensitized Photochemical Cell
- *(High efficiency multi-gap tandem cells)*

## III. 3<sup>rd</sup> Generation ( $n_{\text{theor}} > 31\%$ ; Queisser-Shockley limit)

- Hot electron converters
- Impact ionization cells
- Mid-band PV
- Quantum Dot Solar Cells

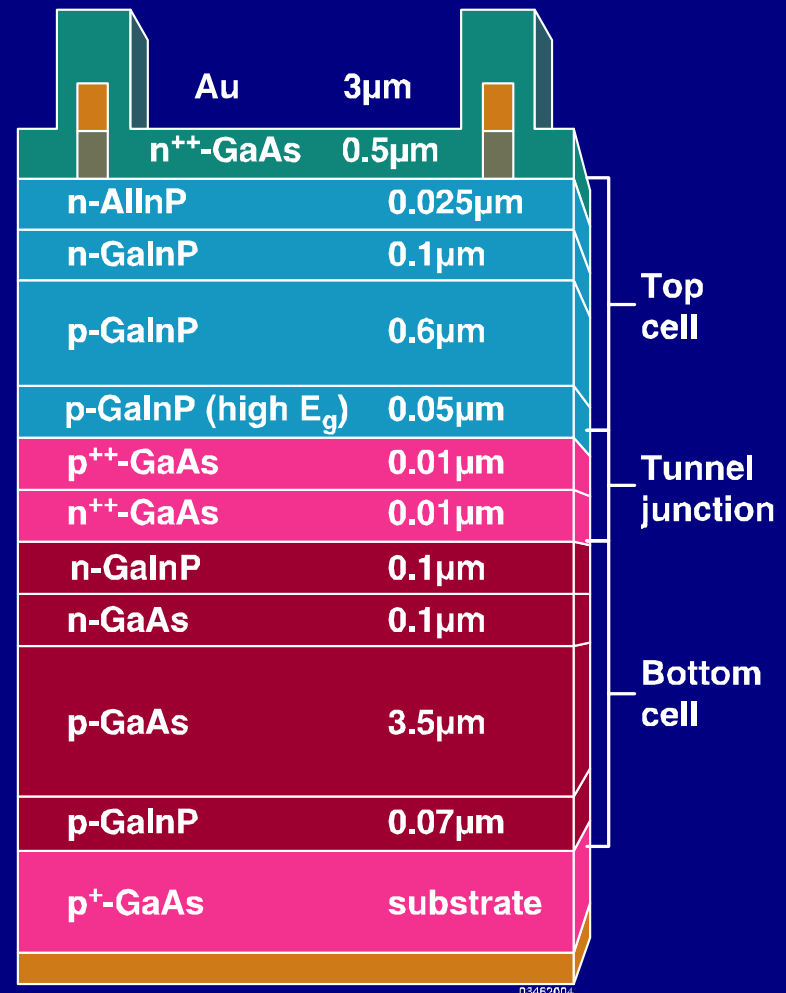


# Integrated Basic Energy Sciences and Photovoltaic Program at NREL Led to the World Record Efficiency Solar Cell

## Several World Record Efficiencies:

- 29.5% 1 sun flat plate cell
- 30.2% 140-180 sun concentrator cell
- 25.7% 1 sun space cell

Gallium Indium Phosphide/Gallium  
Arsenide Photovoltaic Solar Cell



03462004

# GaInP<sub>2</sub>/GaAs Tandem Solar Cells

Terrestrial Power System

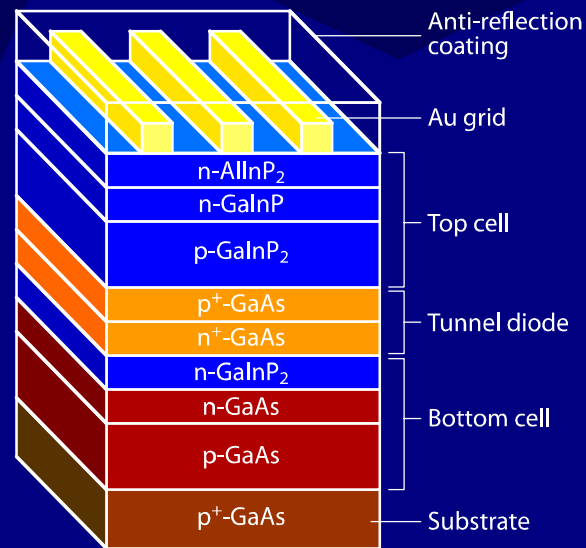


Space Vehicle Power System



## Tandem GaInP<sub>2</sub>/GaAs Device

World record  
29.5% efficiency  
(AM1.5; 1-sun)



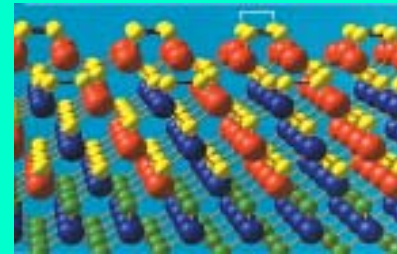
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# Science of Semiconductor Alloys Leads to Record Solar Cell

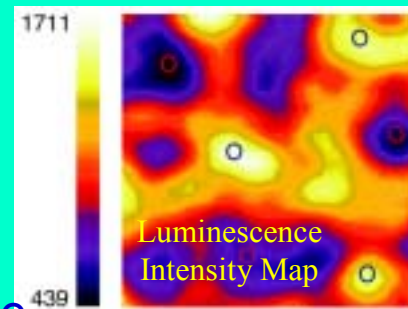
## Studies Relate Spontaneous Ordering in a Semiconductor Alloy to Optoelectronic Properties

- Superstructure ordering modifies energy band structure.
- Allows tailoring optical properties to optimize solar cell performance.
- Resulted in a record-performance “triple junction” photovoltaic device (32.4% efficiency!)
- These devices are being applied in space-based applications and terrestrial light concentrator devices.

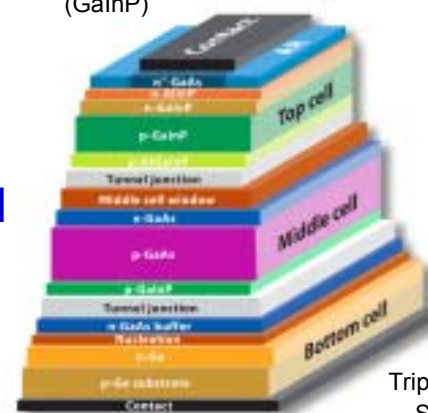
Mascarenhas, Olsen, and Wei, NREL  
with co-funding by DOE/SC/BES and DOE/EERE



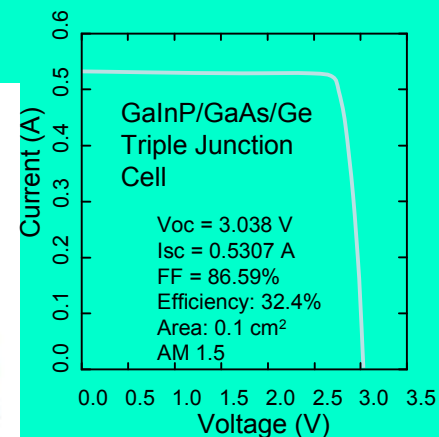
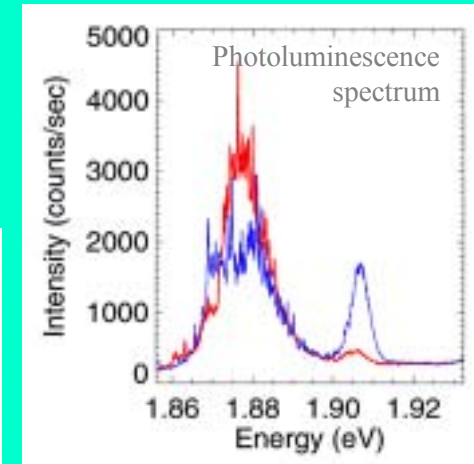
Ordering in GaInP



Ordered Domains  
(GaInP)



Triple-Junction  
Solar Cell



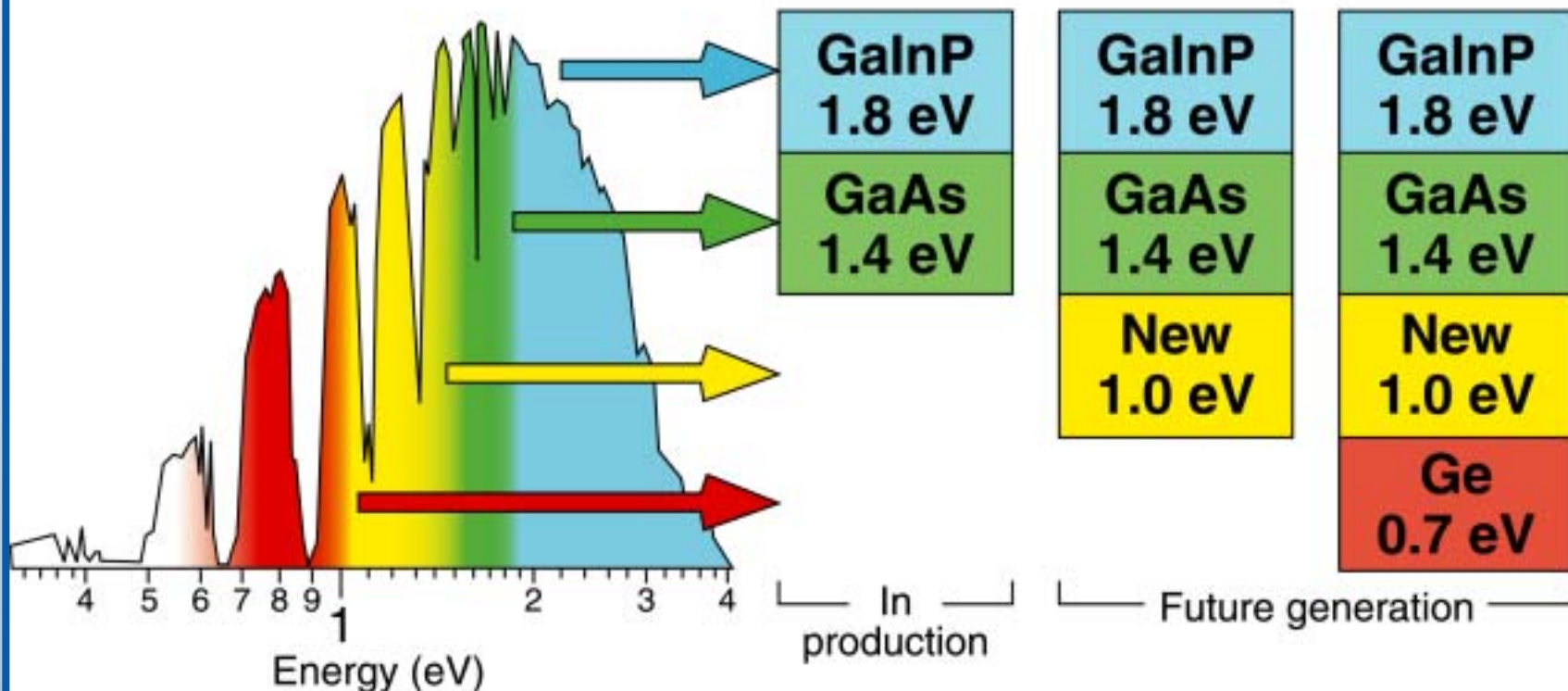
# High Efficiency Multijunction Solar Cells

- Want 1eV material lattice-matched to GaAs

⇒ Try GaInNAs

Calculated efficiencies (ideal)

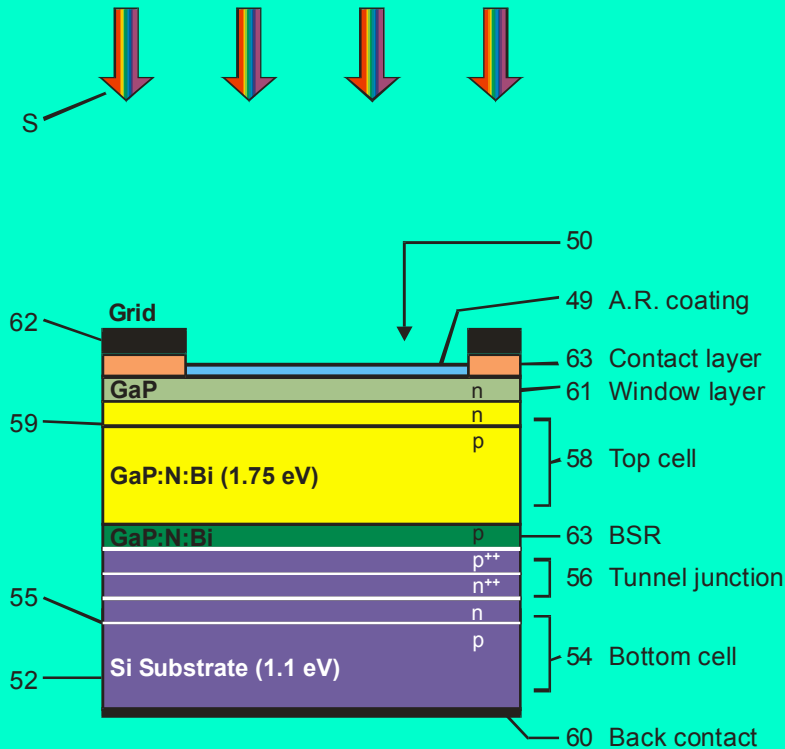
500X AM1.5D:	36%	47%	52%
One sun AMO:	31%	38%	41%



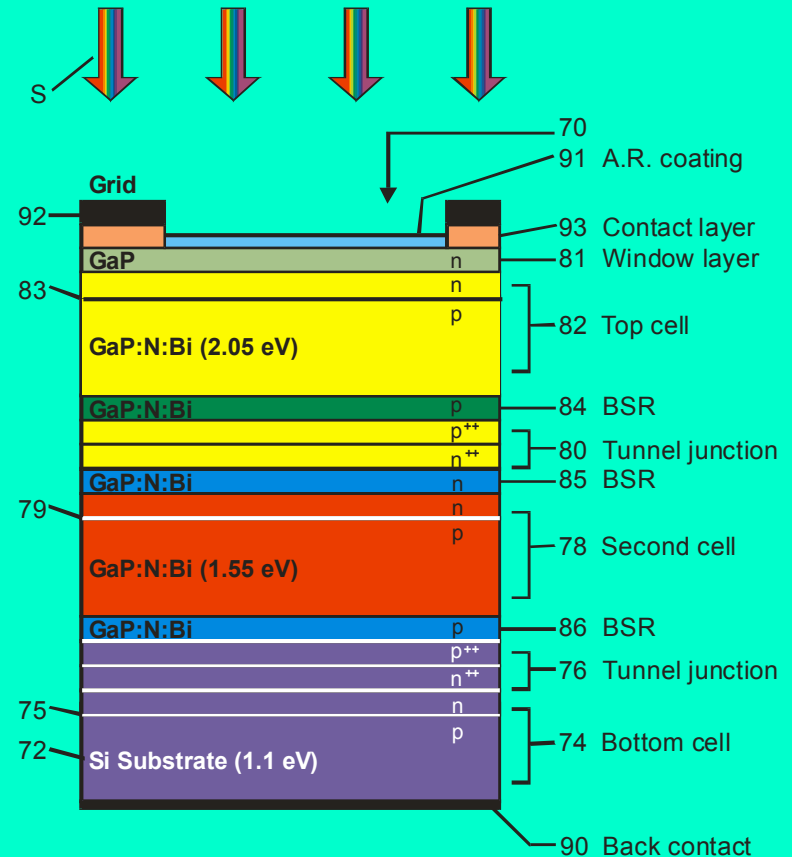
03045405

# Ultimate Solar Cells

AM1 Efficiency  
Theoretical: 36%



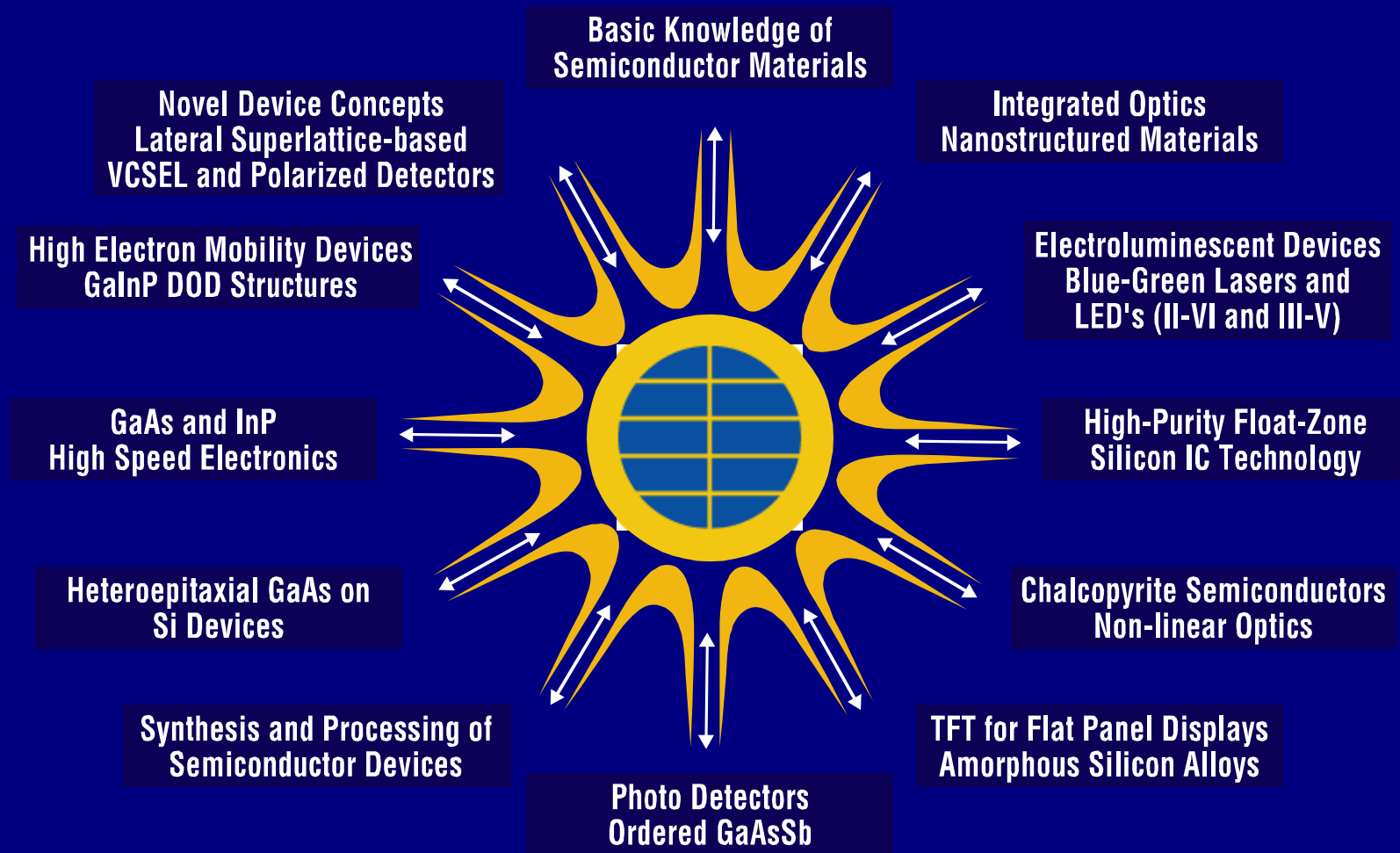
AM1 Efficiency  
Theoretical: 40%





# Synergy Between Photovoltaic & Semiconductor Technologies

Z8.B1496.30





# Chemical Sciences

## Goal

The goal of the Chemical Sciences program at NREL is to advance the basic understanding of the relevant science in chemistry, photochemistry, photoelectrochemistry, catalysis, materials chemistry, and semiconductor physics and chemistry that supports evolving solar photochemical conversion technologies; efforts are also made to integrate the advances in the basic chemical sciences into relevant technology development activities.

## Approaches

- Synthesis and characterization of novel semiconductor quantum structures
- Dye-sensitized TiO<sub>2</sub> solar cells
- Synthesis of new molecular catalysts for C1 chemistry
- Carrier dynamics and quantization effects
- Liquid crystalline and molecular semiconductors
- Nanoscale chemistry of materials

# Summary of NREL's Activities in Nanoscience/Nanotechnology

## Chemical Sciences

Work on colloidal quantum dots began in 1983 under the sponsorship of BES/Chemical Sciences. NREL researchers were among the first to report on quantization effects in nanosize semiconductor particles (1984); over 80 publications on quantization effects and quantized structures have been published in the peer-reviewed literature, including nanostructured solar cells. Current research is focused on III-V semiconductor quantum dots and quantum dot arrays produced by colloidal chemistry.

## Applications

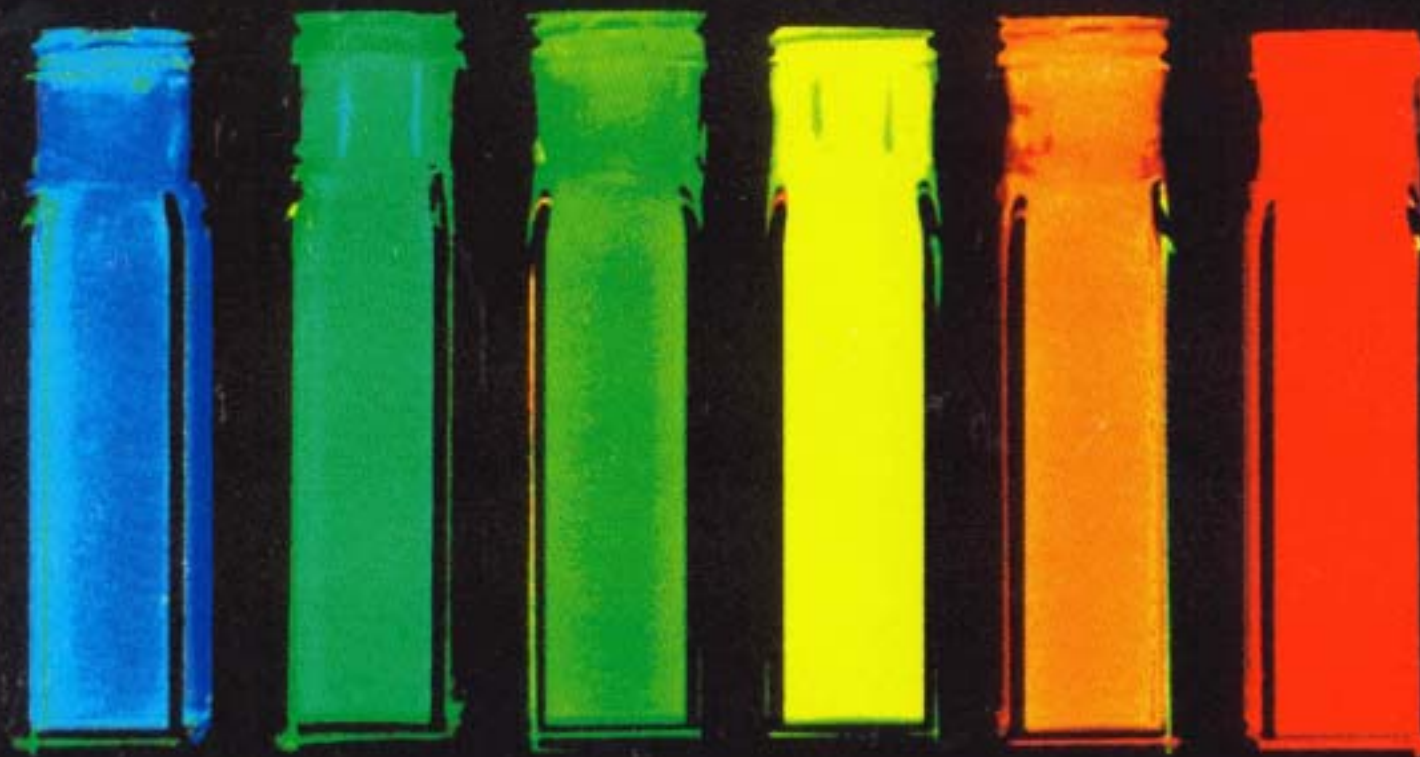
- Novel high efficiency and low cost photovoltaic and photochemical conversion of solar photons to fuels, chemicals, and electricity
  - Quantum dot solar cells
  - Dye-sensitized nanocrystalline photochemical solar cells
- Photocatalysis/photodestruction of pollutants
- Catalysis and fuel production

# Center's Research Activities on Nanoscience/ Nanotechnology Supported by DOE/BES

- Controlled growth and characterization of nanoscale materials (epitaxial, solution, and self-organized growth)
- Synthesis and characterization of carbon-nanotubes (hydrogen storage and separation membranes)
- Biological approach to nanostructure fabrication (interaction with protein)
- Electronic coupling of self-assembled quantum dots (QDs)
- Photo-induced electron transfer between QDs and host materials (sensitized  $\text{TiO}_2$  solar cell)
- QDs for ultra-high efficiency solar cells
- Nanomaterials for catalysis and environmental remediation
- Theory and simulation – electronic structure of QDs

# Consequences of Quantization

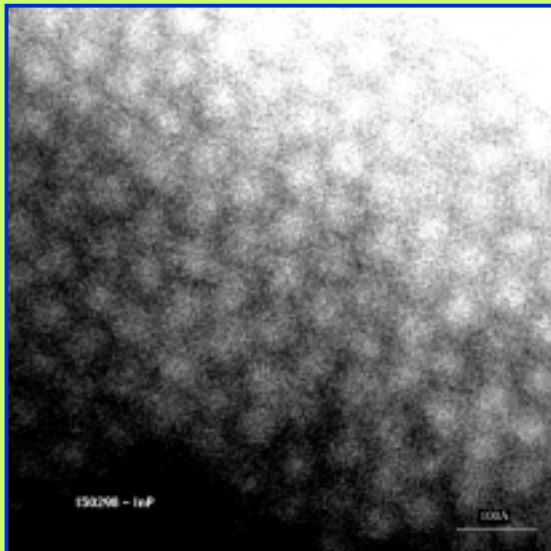
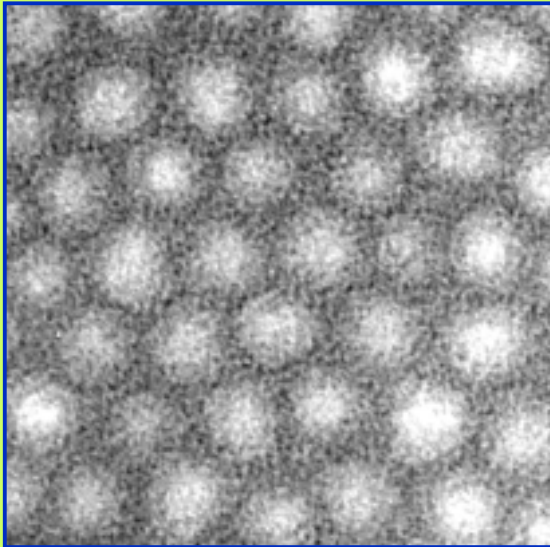
- Dramatic variation of optical and electronic properties
- Large blue shift of absorption edge
- Discrete energy levels/structured absorption and photoluminescence spectra
- Enhanced photoredox properties for photogenerated electrons and holes
- **Greatly slowed relaxation and cooling of photogenerated hot electrons and holes**
- **PL blinking in single QDs**
- **Enhanced Inverse Auger (impact ionization)**
- Conversion of indirect semiconductors to direct semiconductors or vice versa
- Greatly enhanced exciton absorption at 300 K
- Greatly enhanced oscillator strength per unit volume (absorption coefficient)
- Greatly enhanced non-linear optical properties
- Greatly modified pressure dependence of phase changes and direct to indirect transitions
- Efficient anti-Stokes luminescence



*Quantum Confined Luminescent (CdSe)ZnS  
Core-Shell Nanocrystals*

03401615

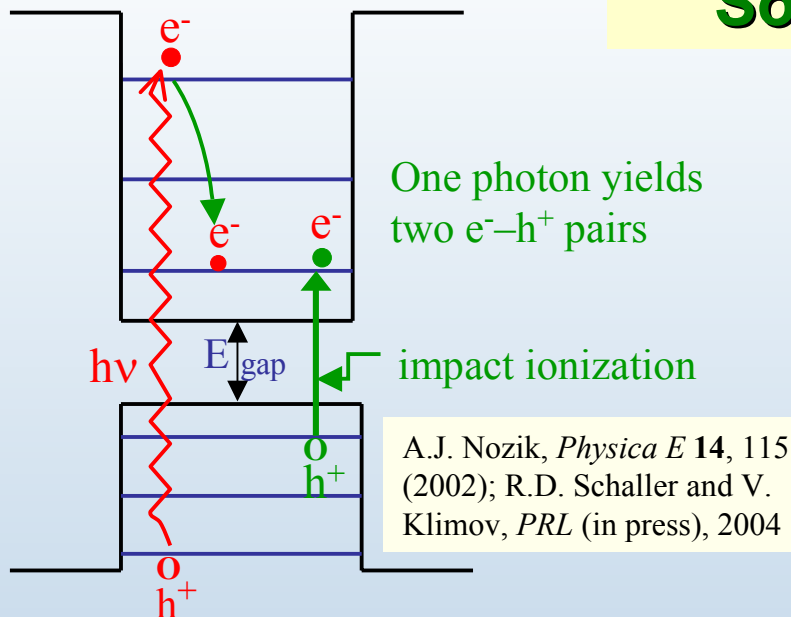
## InP Nanoparticle Arrays



TEM of hexagonal ordered array of ~50 Å diameter colloidal InP QDs. Top panel: 2D ordered array. Bottom panel: Ordered array shows multiple layers and a step to a single layer.

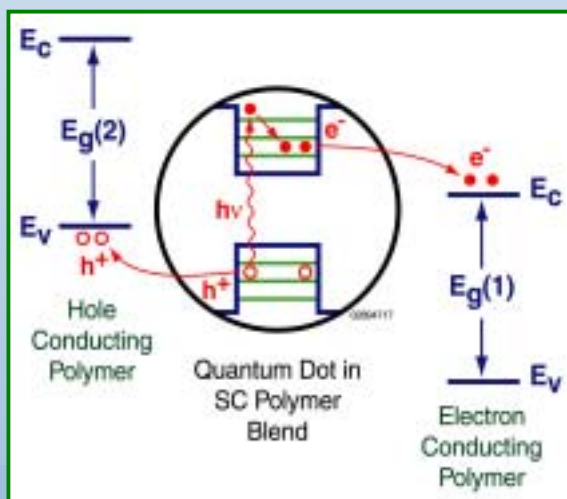
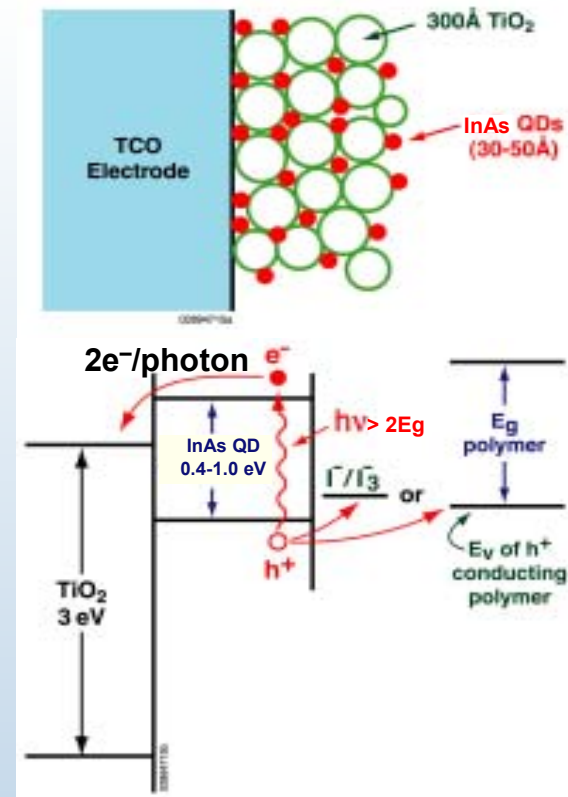


## Enhanced Photovoltaic Efficiency in Quantum Dot Solar Cells by Inverse Auger Effect (Impact Ionization)



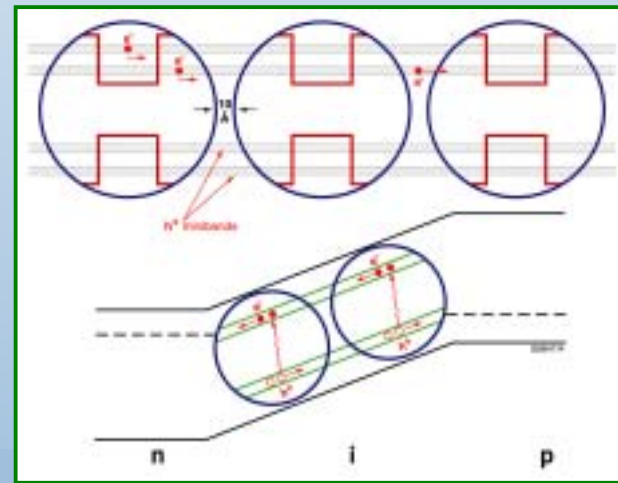
## Quantum Dot Solar Cells

### QD-Sensitized Nanocrystalline $\text{TiO}_2$ Solar Cell

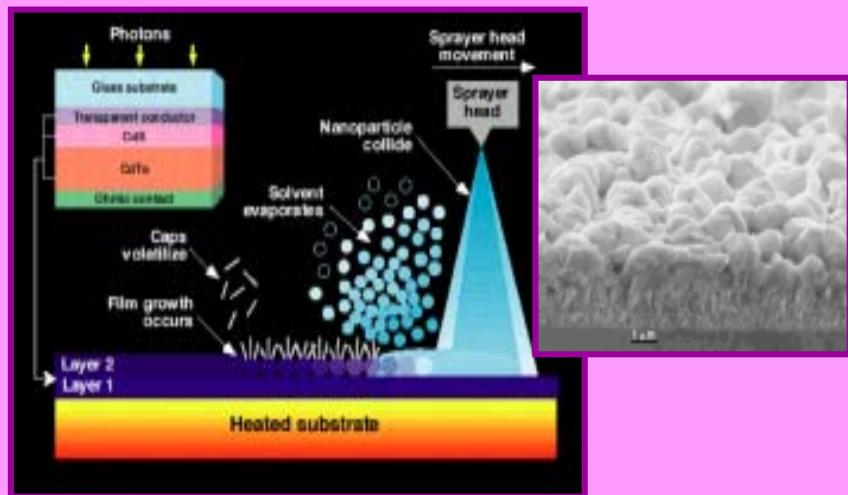


### QD-Conducting Polymer Blend Solar Cell

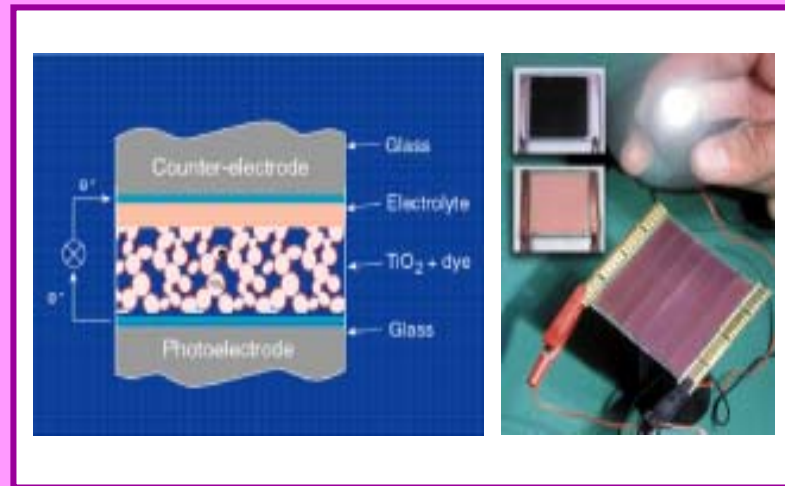
### p-i-n QD Array Solar Cell



# Novel PV Concepts and New Materials— Research Issues and Directions



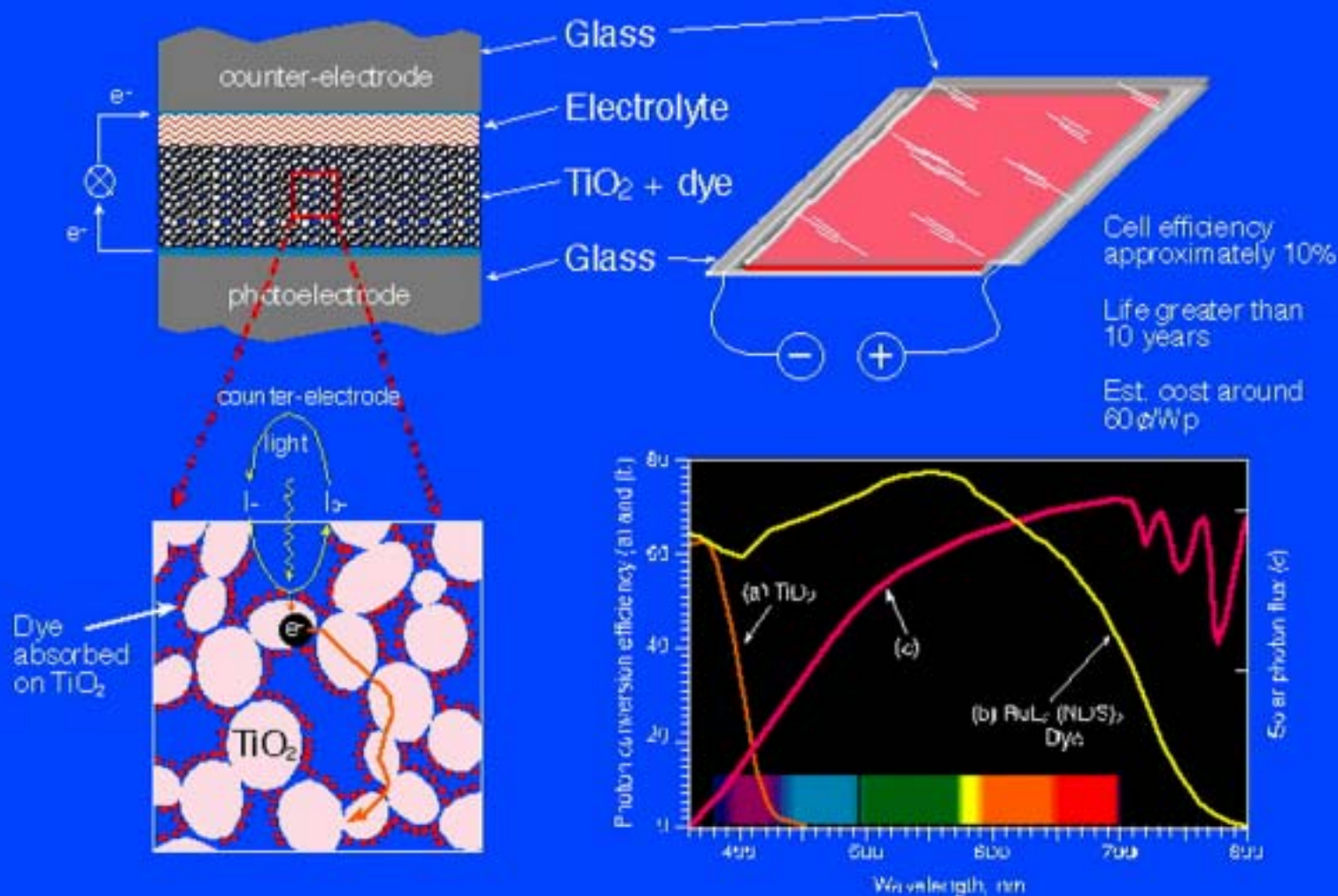
- **Nanoparticle-derived precursors for PV**
- Potential for very low cost
- Low process temperatures, non-vacuum
- Potential for smooth, dense films
- Absorbers (CdTe, CIS, ...)
- Transparent conductors ( $\text{SnO}_2$ , CdS, ...)
- Contacts (Ag, Au, Pt, ...)
- Nanocrystals, nanotubes, nanorods
- Nanocharacterization



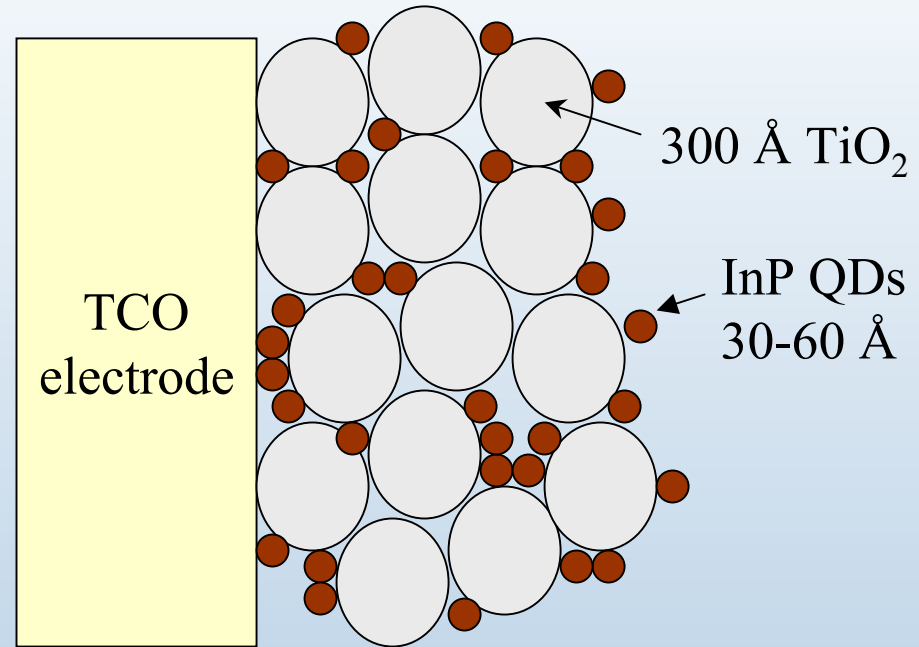
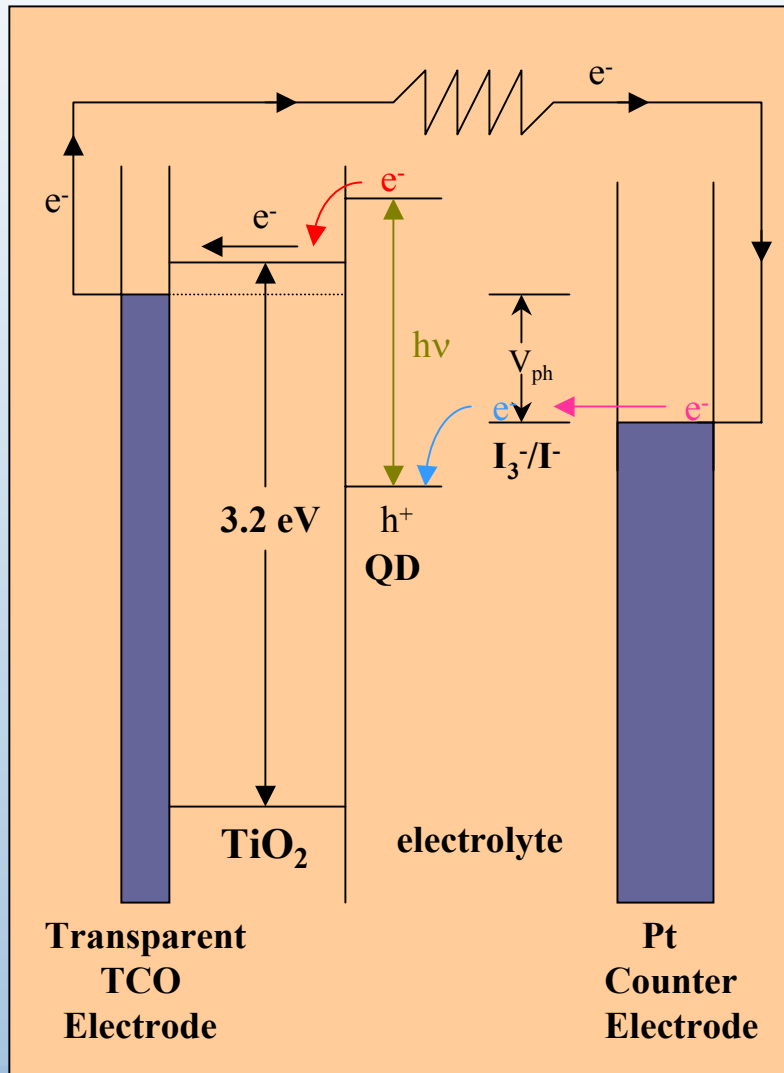
- **Dye-sensitized  $\text{TiO}_2$  photochemical cells**
- Potential for very low cost
- Nanocrystalline  $\text{TiO}_2$ , with monolayer dye sensitizer, in liquid electrolyte
- 11%-efficient cell; scale-up for consumer products underway
- Dye stability issue
- Gel or solid-state electrolytes in research



# Dye Sensitized TiO<sub>2</sub> Solar Cell



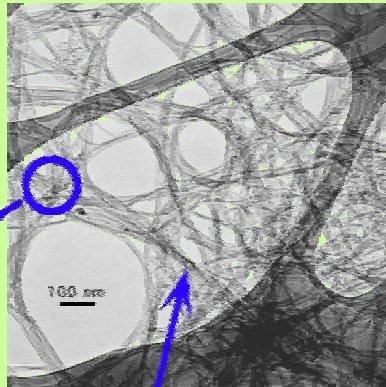
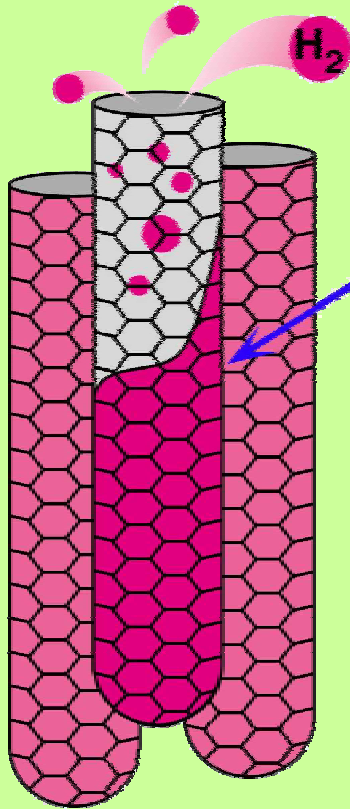
# Quantum Dot Sensitized TiO<sub>2</sub> Solar Cell



- Analogous to dye-sensitized TiO<sub>2</sub> solar cells
  - 10 to 20  $\mu\text{m}$  film of NC TiO<sub>2</sub> (10-30 nm)
  - Ru dyes  $\Rightarrow$  Efficiency  $\sim$  11%
- Advantages of QD's as sensitizers:
  - possibility of slowed hot  $e^-$  cooling
  - possibility of impact ionization
  - tunable absorption

# Hydrogen Research

Hydrogen from photoelectrochemical  
splitting of water



Carbon nanotubes  
for storage

Mutant algal strains used to split water  
and produce hydrogen in the photobioreactor  
pictured in the background



06225



03595 Laboratory

# ***Hydrogen: A National Initiative***

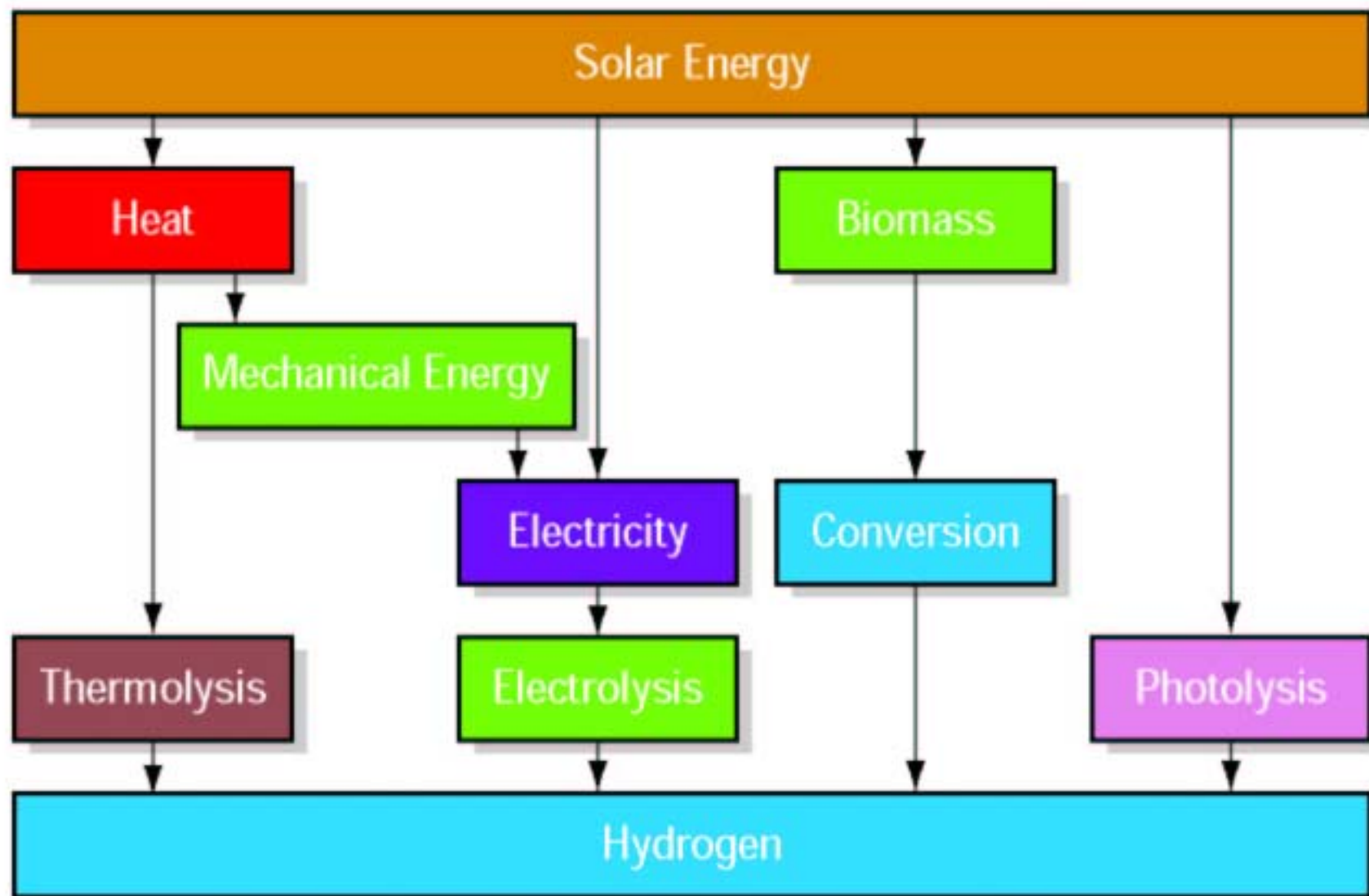
**“Tonight I’m proposing \$1.2 billion in research funding so that America can lead the world in developing clean, hydrogen-powered automobiles... With a new national commitment, our scientists and engineers will overcome obstacles to taking these cars from laboratory to showroom, so that the first car driven by a child born today could be powered by hydrogen, and pollution-free.”**

**President Bush, State-of-the-Union Address,  
January 28, 2003**



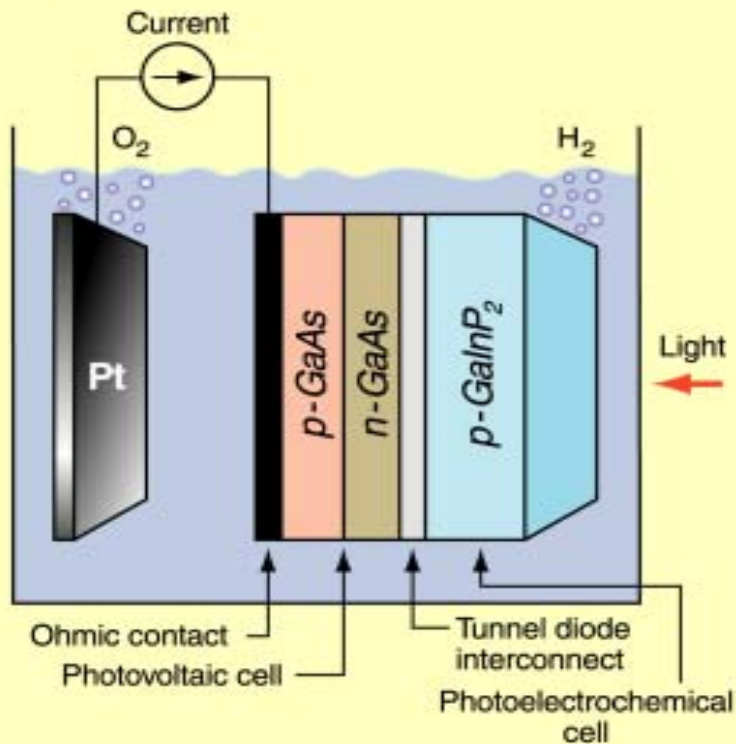


# Sustainable Paths to Hydrogen



# World Record Photoelectrolysis Device Science, April 17 1998.

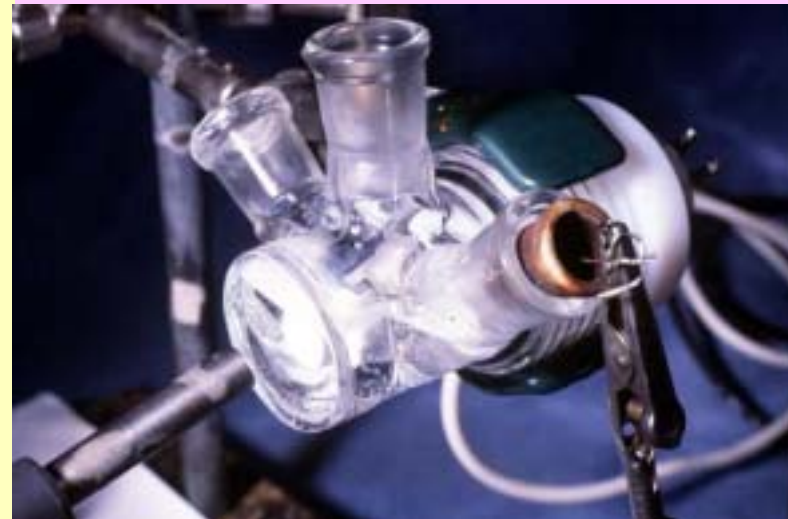
Novel cell uses light to produce  $H_2$  at 12.4% efficiency



**Note:** *n* and *p* refer to *n*- and *p*-type semiconductors

**Credit:** Adapted with permission from Science, copyright 1996 AAAS

- Direct water electrolysis.
- Unique tandem (PV/PEC) design.



## Experimental Cell

# Biological Sciences

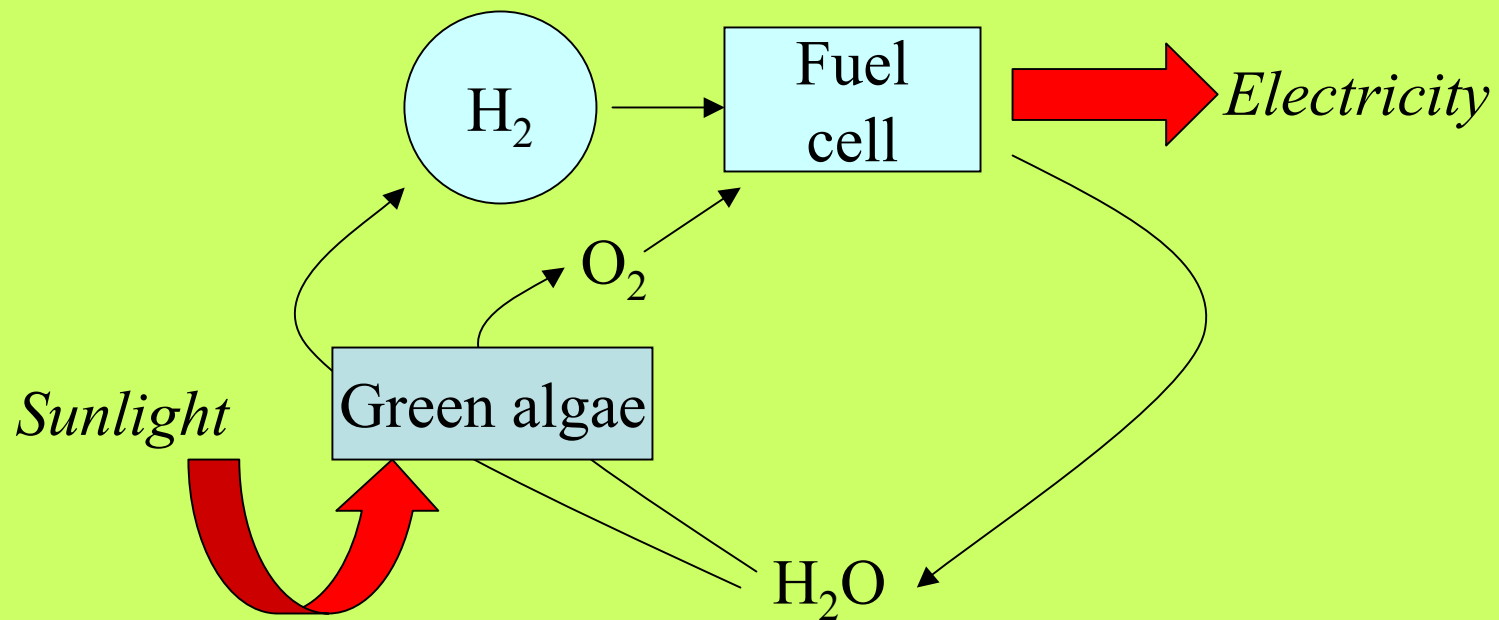
## Goal

The goal of the Biological Sciences program at NREL is to advance basic understanding of bacterial and plant photosynthesis, including relevant metabolic pathways, and to apply that knowledge to develop renewable fuels, chemicals, and materials, as well as address environmental problems.

## Approaches

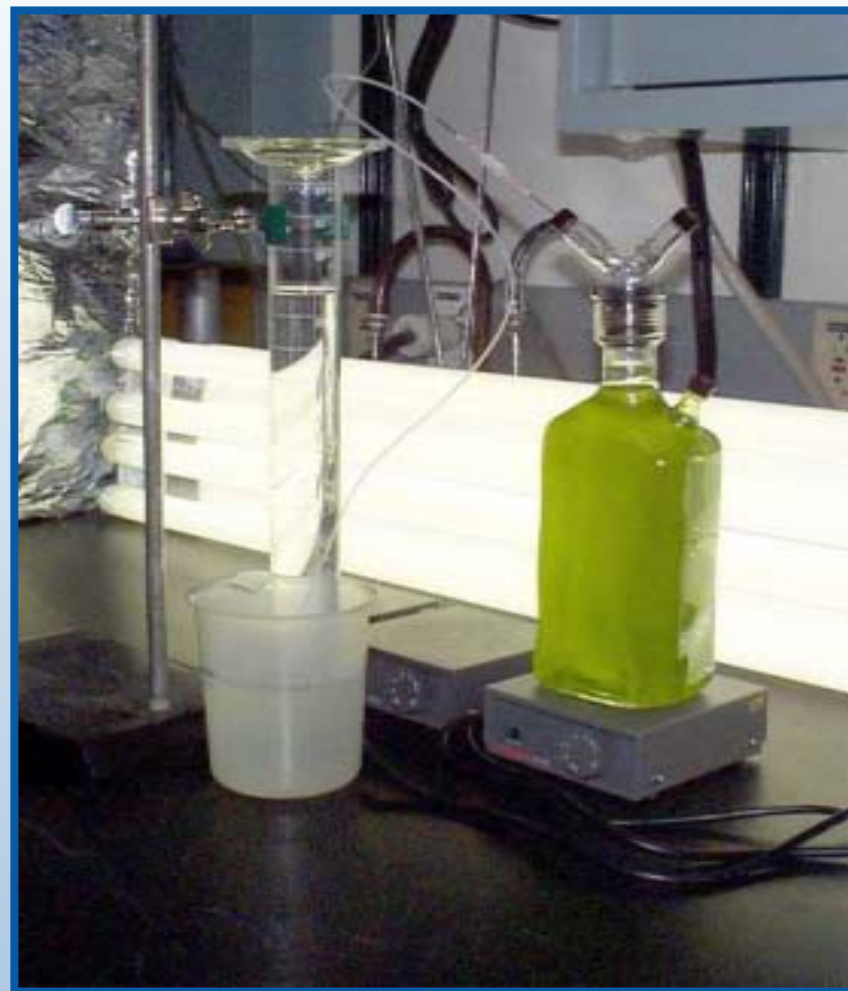
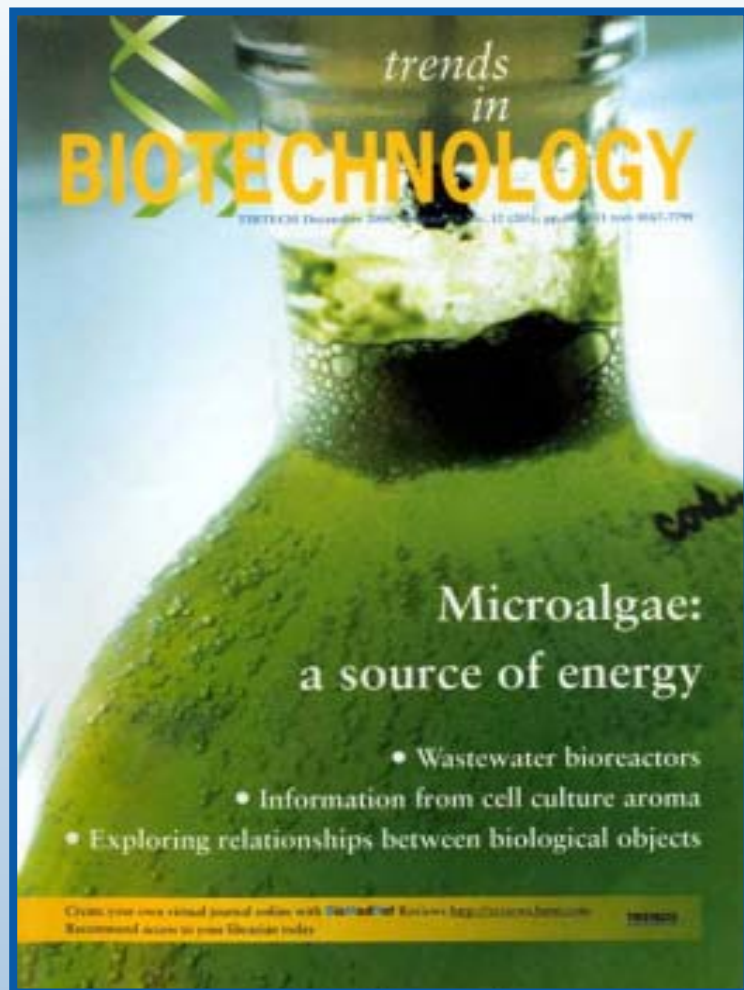
- Basic studies of photosynthetic water-splitting in plants and algae
- Regulating H<sub>2</sub> and CO<sub>2</sub> metabolism in algae

# RENEWABLE HYDROGEN PRODUCTION/UTILIZATION





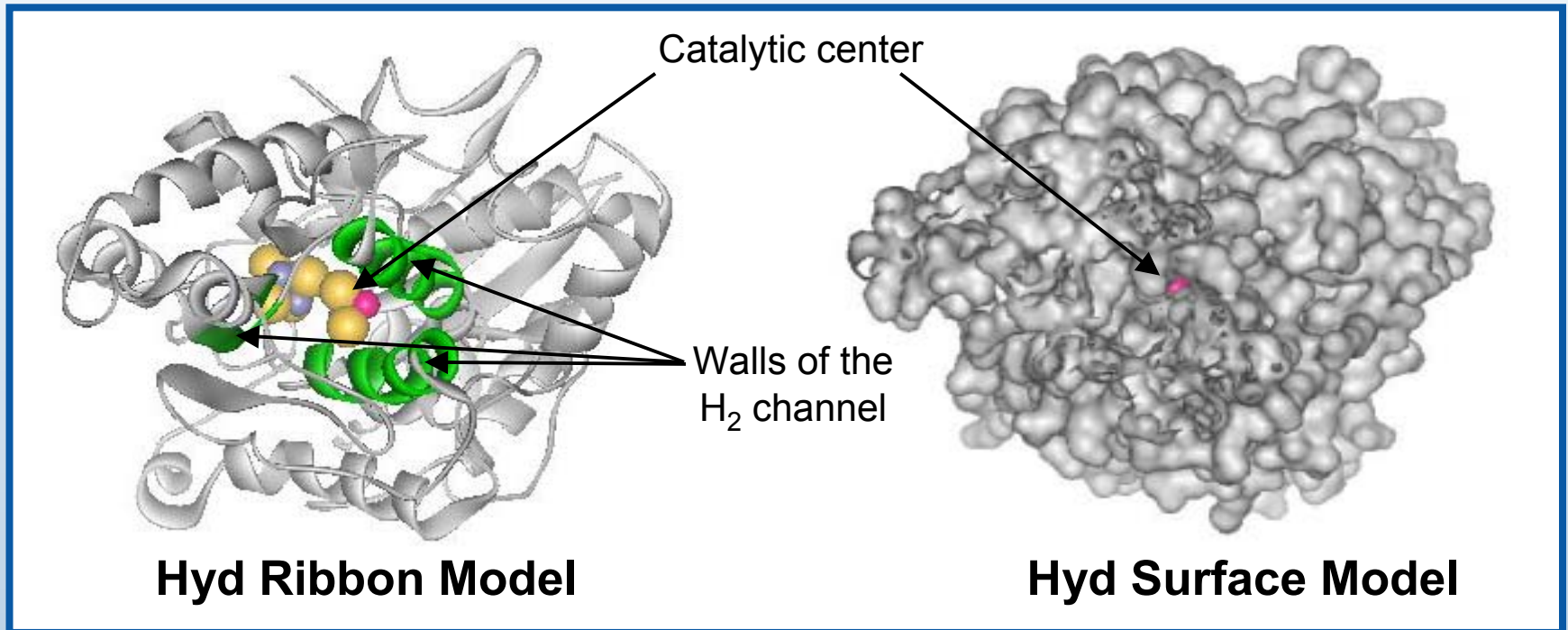
# A Novel Algal H<sub>2</sub>-Production System



H<sub>2</sub> being produced by *Chlamydomonas*

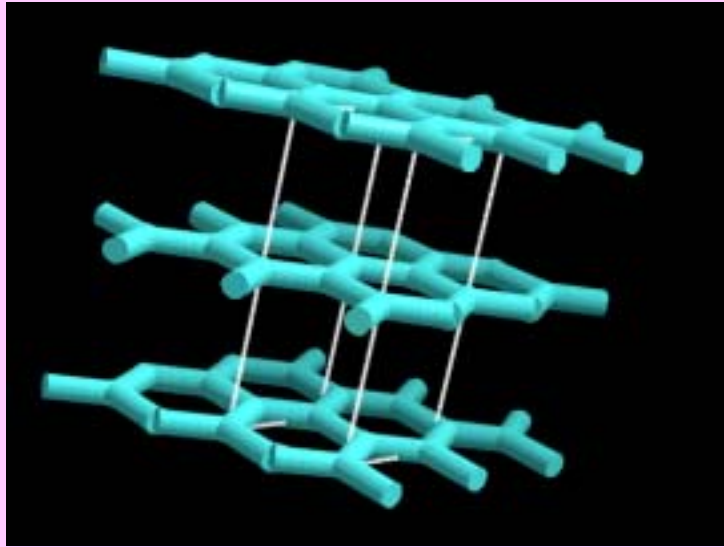
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# Biohydrogen by Engineering an O<sub>2</sub>-Tolerant Hydrogenase

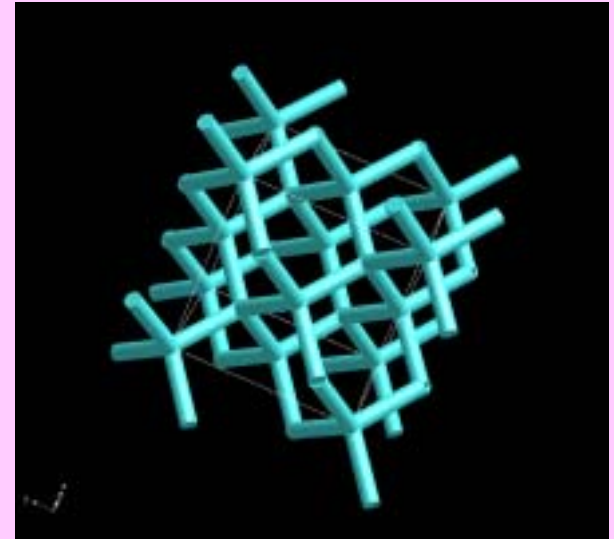


**Molecular Engineering:** Detailed structural modeling of the Hyd proteins is allowing us to develop a knowledge-based means to genetically engineer O<sub>2</sub> tolerance into algal hydrogenases.

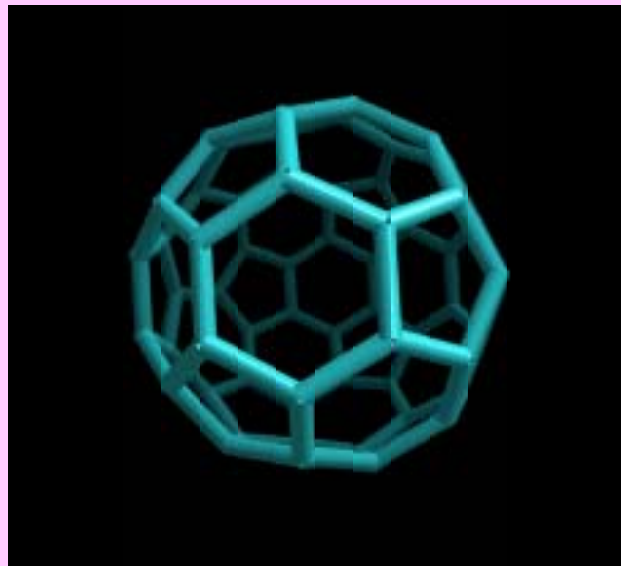
# Graphite



# Diamond

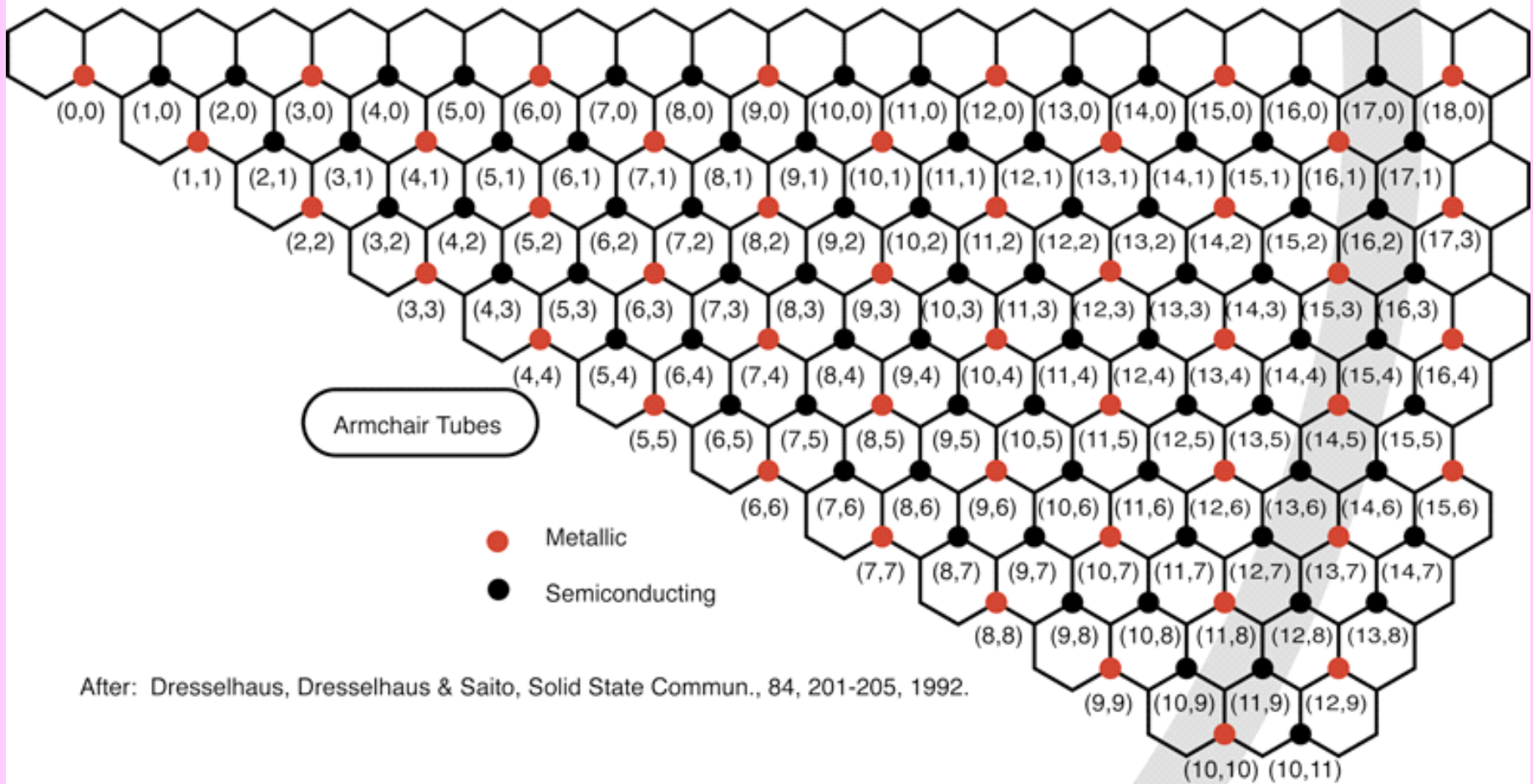


# $C_{60}$



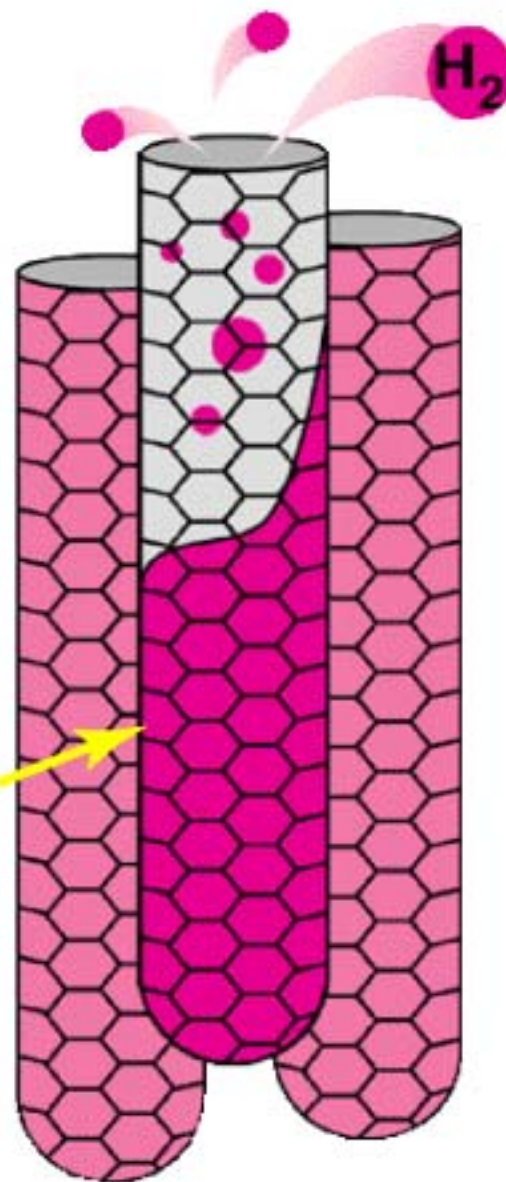
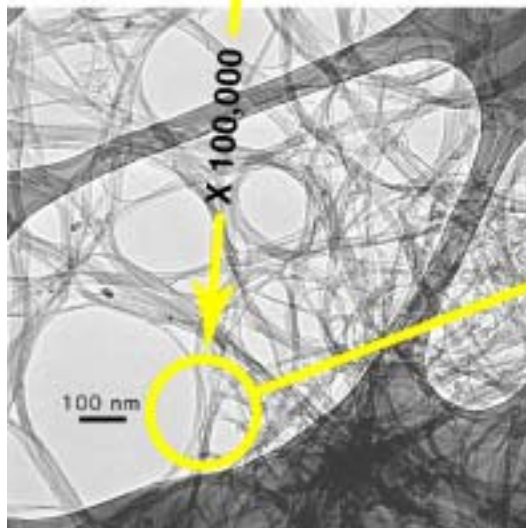
# Zig-Zag Tubes

~ 1.4 nm Diameter Tubes

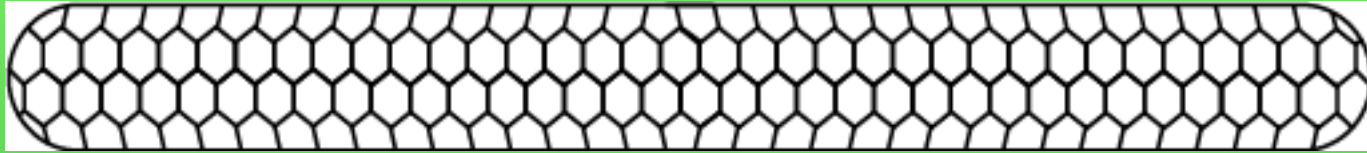


After: Dresselhaus, Dresselhaus & Saito, Solid State Commun., 84, 201-205, 1992.



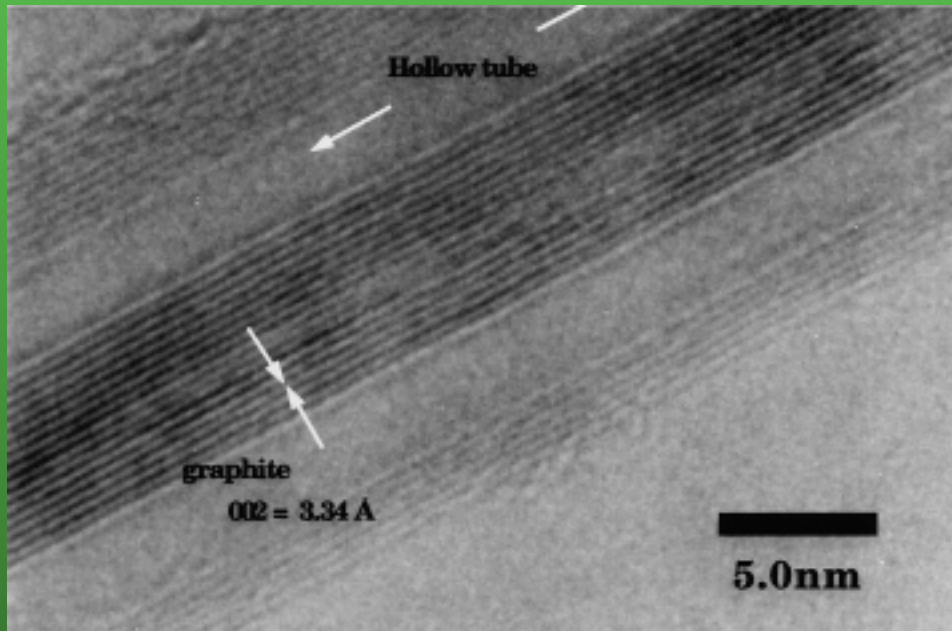


# Single-wall Carbon Nanotubes



Single sheet of graphite wrapped into a tube: microns in length,  $\sim 1\text{-}2$  nm diameter, capped.

# Multi-wall Carbon Nanotubes



Concentric cylinders of graphite with a hollow center, capped.

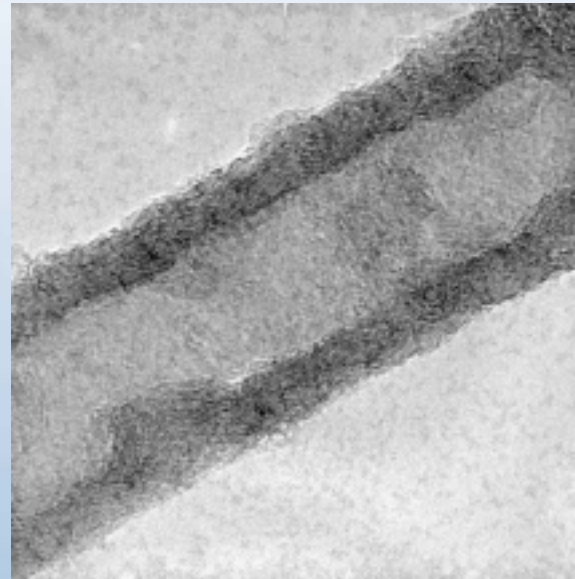
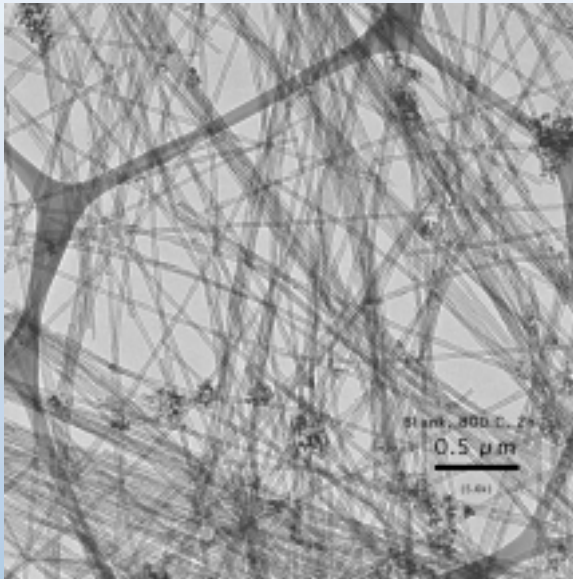
Spacing between each cylinder is similar to the inter-planar spacing in graphite.

Generally 2-50 shells, microns in length.

Inner and outer diameters are typically 2-10 and 15-50 nm.

# Template-synthesized Carbon Nanotubes

several layers of poorly graphitized carbon  
with limited domain size.



# SWNT Technologies

- Hydrogen storage
- Gas separation membranes
- Rechargeable Li Ion batteries
- Electrically conducting polymer and ceramic composites
- Ultracapacitors
- High-strength, high-temperature, low-weight composites
- Energy absorbing armor
- Heat dissipation / shielding
- Nanoscale wires & interconnects
- Electromagnetic shielding
- Artificial muscle
- Field emission displays
- Chemical and Biological sensors
- Toxic gas adsorbents

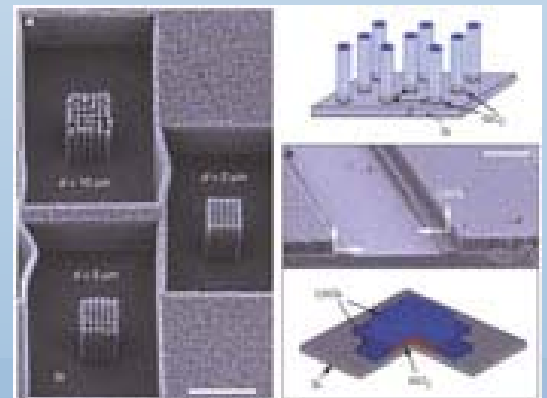
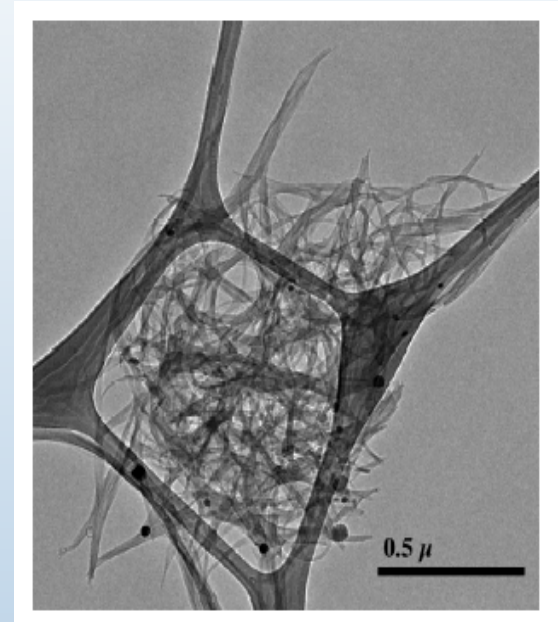


# Single-Wall Carbon Nanotubes

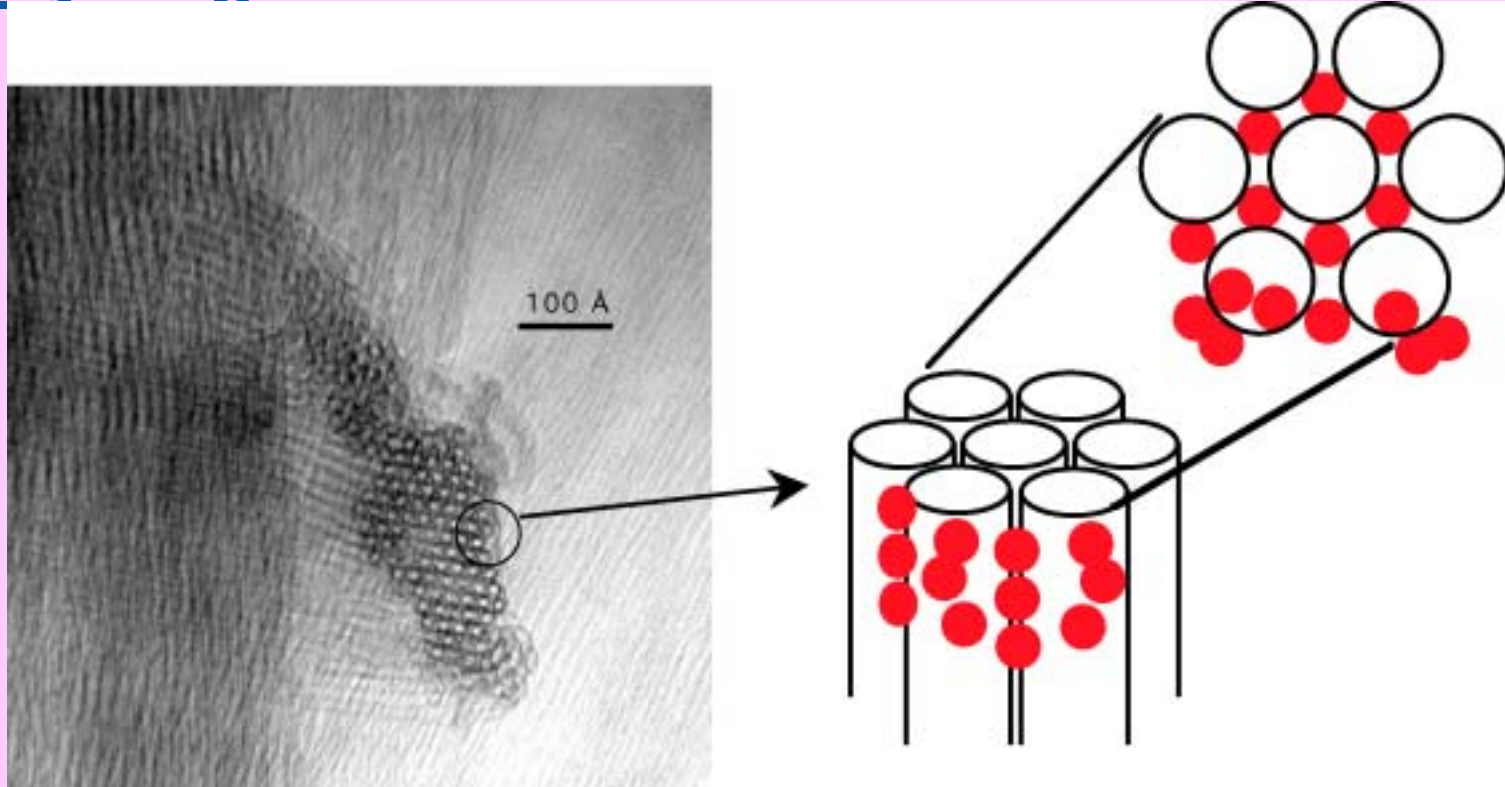
- Capacity around 4 wt%
- Doped SWNTs to 7 wt% by NREL
- Ambient temperature, moderate pressure
- SWNTs are made by arc discharge, laser vaporization, CVD, and lithographically
- SWNTs must be purified, cut, and the ends opened

***Reproducibility is a critical issue.***

*Wei, B. Q., et al, Nature, Vol. 416, April 2002*



# SWNTs: An Ideal Adsorbent for Hydrogen?



**Non-dissociative adsorption of H<sub>2</sub> at near ambient conditions.  
Heat of adsorption = 19.6 kJ/mol.**

A.C. Dillon, K.M. Jones, T.A. Bekkedahl, C.H. Kiang, D.S. Bethune, & M.J. Heben, *Nature* (386) 377, 1997.

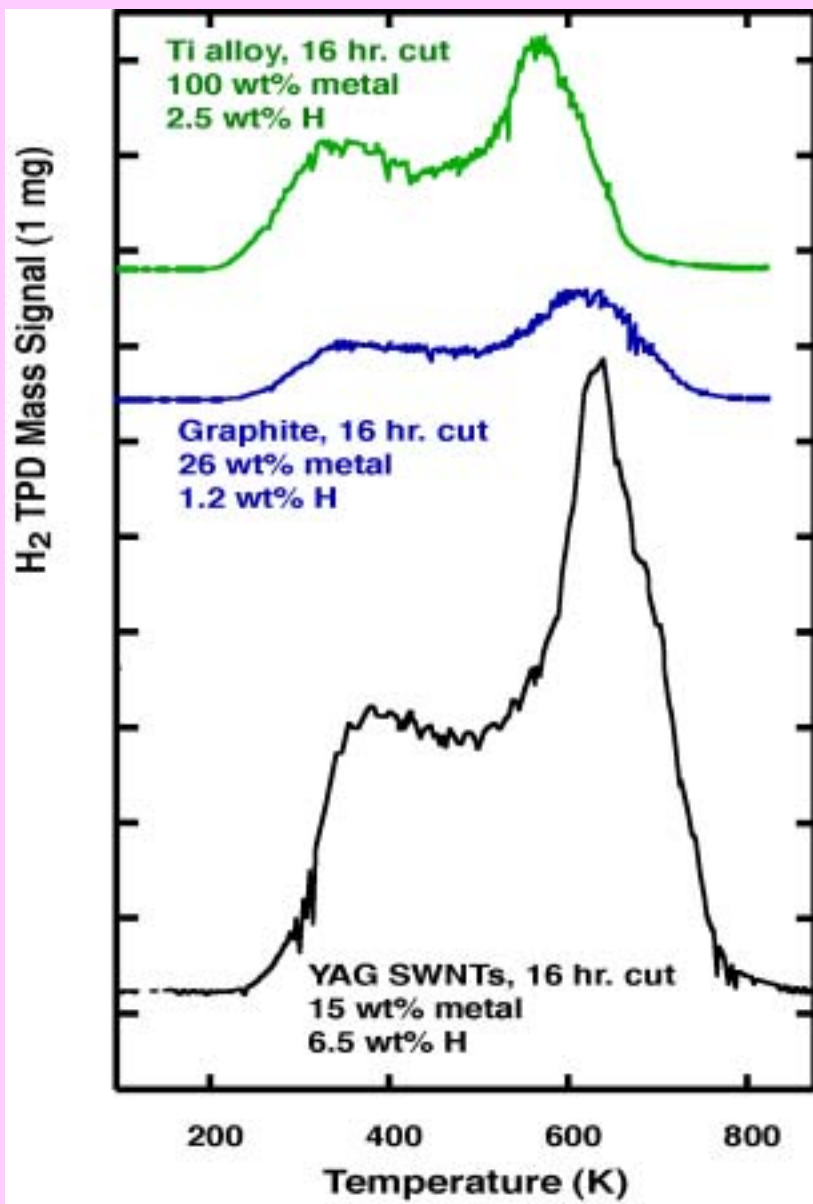
## Metal Facilitated Hydrogen Storage in Graphitic Carbon Materials

Hydrogen exposures are ~5 min. at room temperature and 500 Torr.

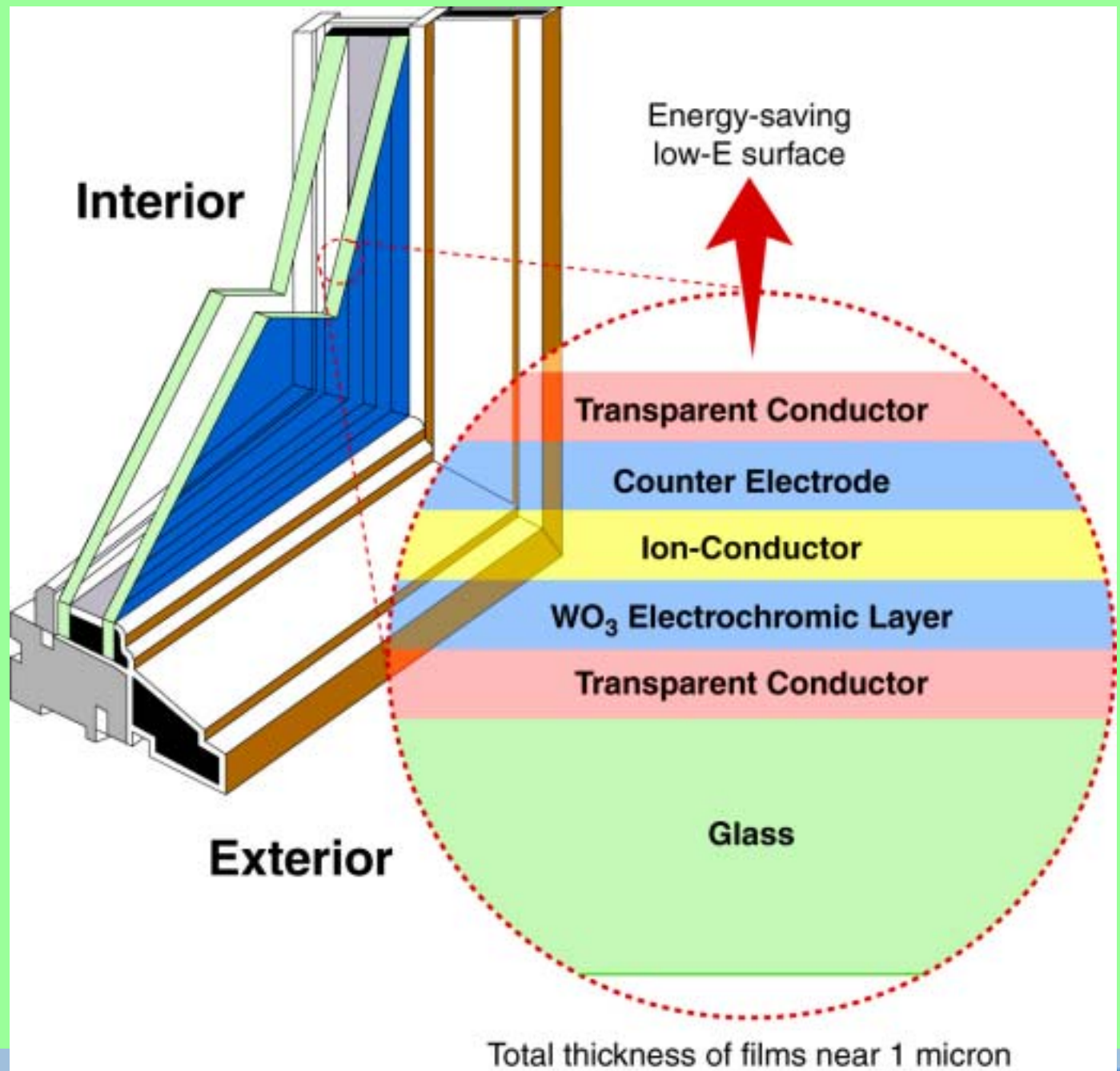
Ti6Al4V alloy is a metal hydride that can store hydrogen at ~2.5-3.0 wt%.

It also appears to activate  $H_2$  storage on graphitic carbon materials.

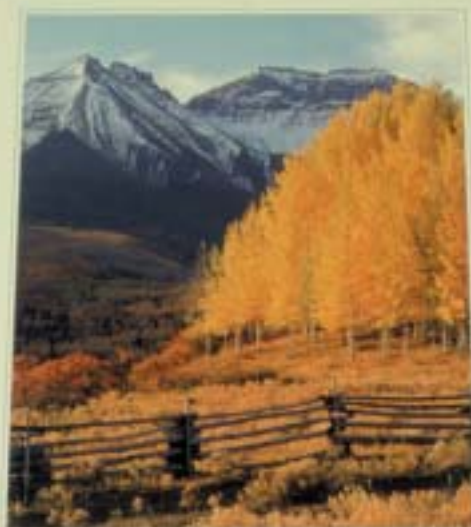
Mixtures of the metal alloy with both graphite and SWNTs results in overall hydrogen storage capacities that are much greater than what would be observed for the alloy alone.



\*NREL



LSI



Golden Mountain Hotel, Golden, Colorado, 1900

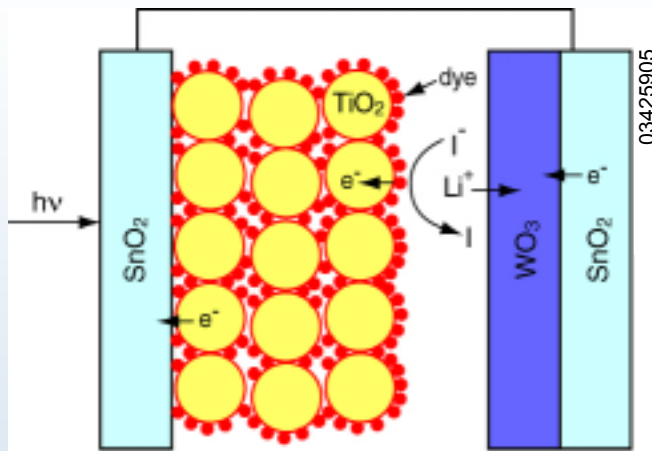


LSI-50



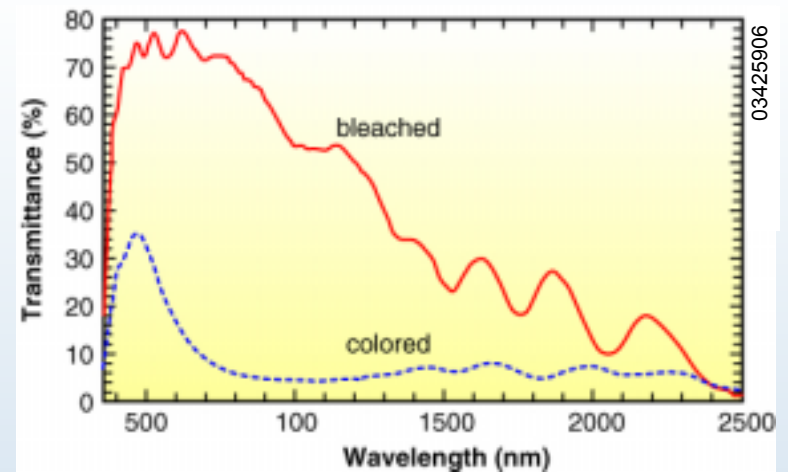




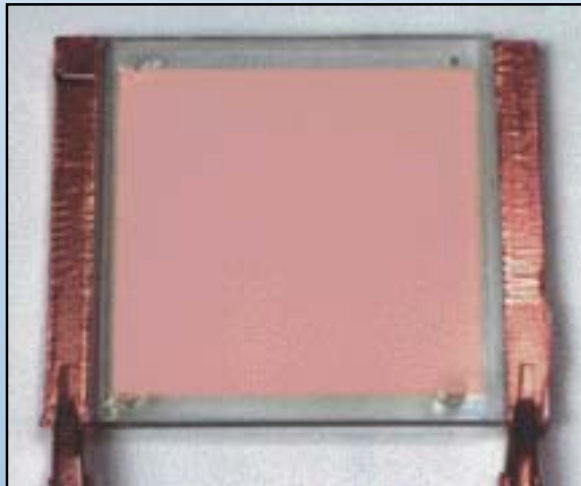


Schematic diagrams of a dye-sensitized electrochromic smart window.

*B.A. Gregg, Endeavour Vol. 21(2) 1997.*



Transmittance spectra of an experimental solid-state electrochromic cell in both the bleached and colored states.

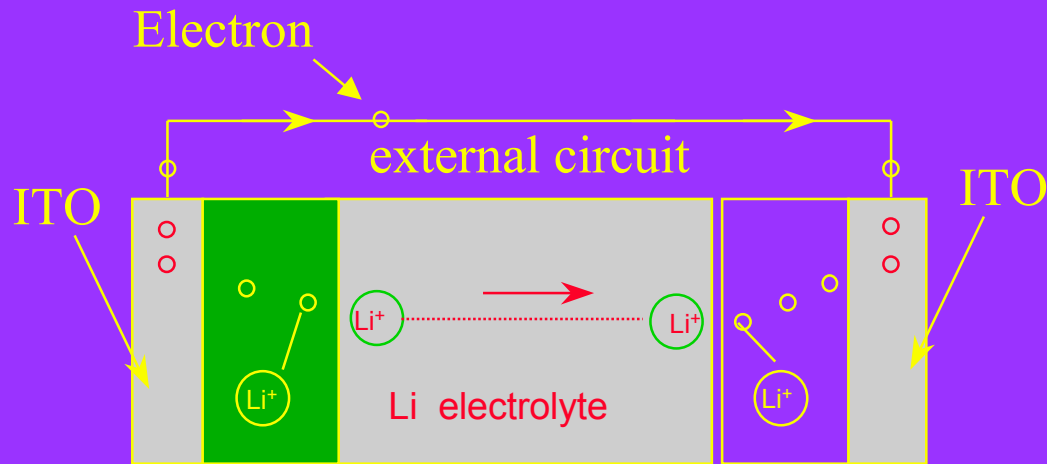


**Bleached**



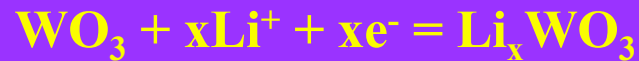
**Colored**

# Typical Electrochromic Device



**Working electrode :**  
a-WO<sub>3</sub>

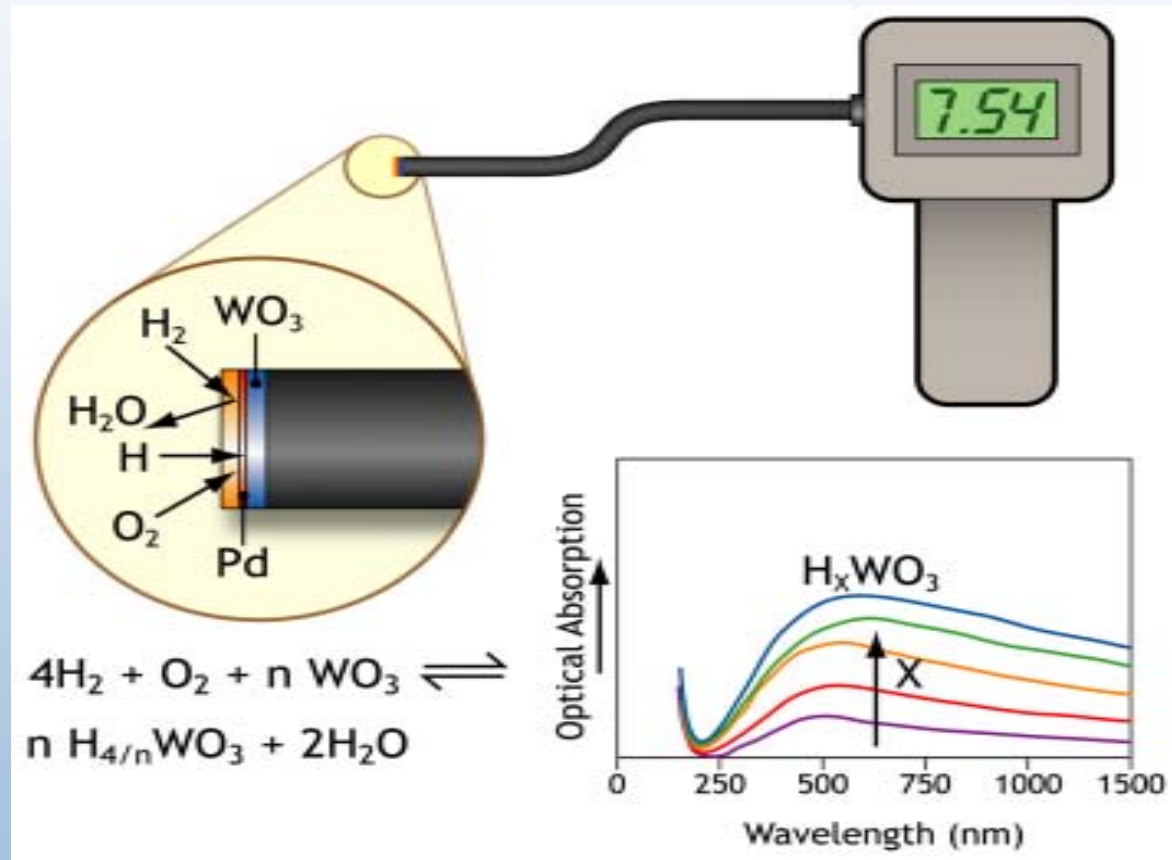
**Counter electrode :**  
V<sub>2</sub>O<sub>5</sub>, NiO<sub>x</sub>



→  
**Coloration**

# Chemochromic Hydrogen Sensors

Roland Pitts  
Ping Liu  
Dave Smith  
Se-Hee Lee  
Ed Tracy



# Program Objectives

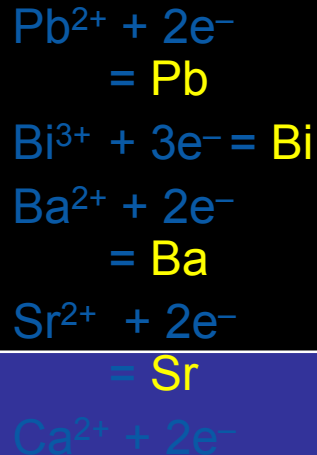
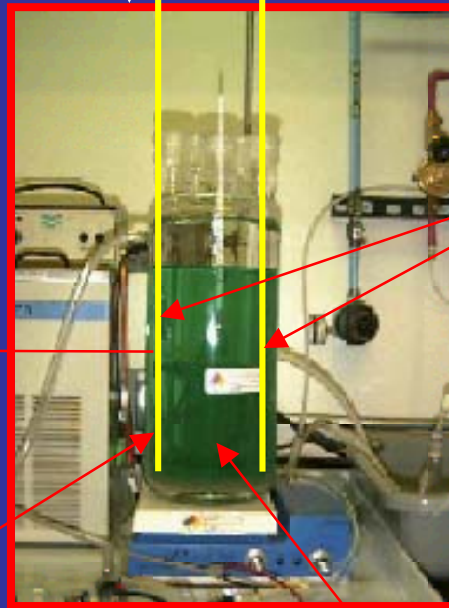
- The U.S. Department of Energy's vision is, "Low-cost, high performance YBCO coated conductors will be available in 2005 in kilometer lengths. For applications in liquid nitrogen, the wire cost will be less than \$50/KA-m, while from applications requiring cooling to temperature of 20–60 K the cost will be less than \$30/kA-m."
- One of the important critical needs to achieve this goal is to develop a simple low-cost technology for producing HTS and also buffer layer for Ni-alloy substrates.
- NREL's project offers non-vacuum electrodeposition and spray deposition processing technology, which is a potentially low-cost, long length, continuous process. At present, we are working on development of both HTS and buffer layer employing electrodeposition and spray deposition process.
- At NREL, we are able to prepared very high-quality electro-deposited superconductor films. The electrodeposited films produced results which are competitive with the best vapor-deposited (e.g., sputtering, evaporation, PLD) HTS.

# Electrodeposition Process

**Electrical variables:**  
overpotential, ...)

- Potentials (V) (half-cell potential, overpotential, ...)
- Current (I)
- Coulombs (C)

$e^-$   $- +$



**Electrode variables:**

- Material
- Surface area
- Geometry
- Surface condition

**Electrical variables:**

- Mode (diffusion, convection)
- Surface concentration
- Adsorption

**Solution variables:**

- Bulk concentration of electroactive ( $C_O$ ,  $C_R$ )
- Concentrations of other species (electrolyte, pH, ...)
- Solvent

# Why Employ the Electrodeposition Process

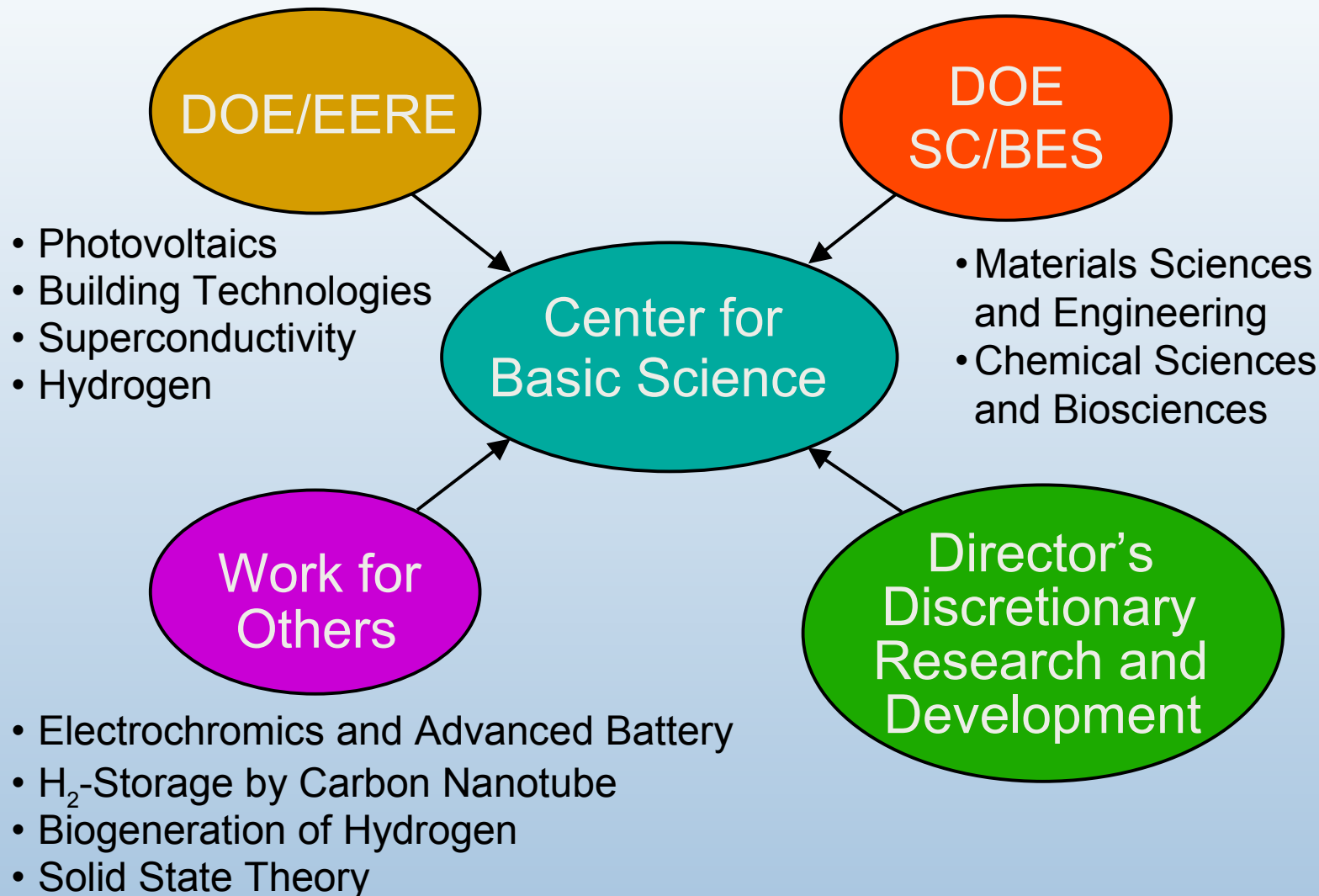
- Electrodeposition offers a potential low cost, high rate, continuous, multi-component deposition process.
- Relatively simple equipment and thus low-cost capital equipment required for large scale commercial investment.
- Controlled deposition rates and effective material utilization.
- Minimum waste generation (solution can be recycled).



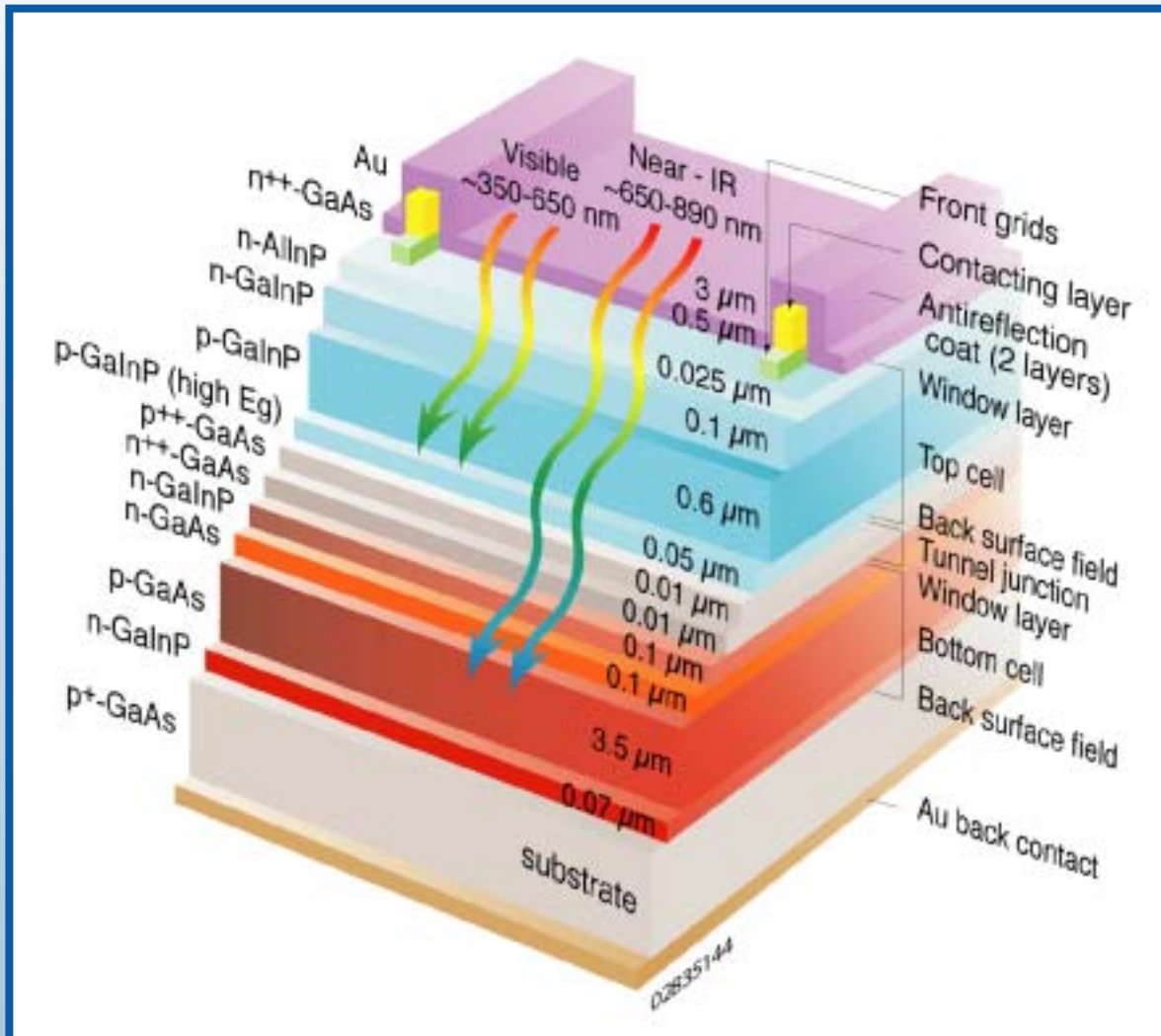
# Conclusions

- The cutting-edge research conducted at NREL provides crucial scientific base underpinning renewable energy technologies.
- Synergism between BES supported basic research and the energy technology programs supported by EERE and co-location of programs at NREL led to outstanding successes in technology development and transfer to industries.
- Our outstanding record of scientific accomplishments through research supported by BES and EERE has made NREL the premier research institution in the field of renewable energy in the world.
- The BES funded research enabled NREL to support a large number of post-doctoral and visiting scientists who have made major contributions to our program as well as providing trained manpower to the nation.

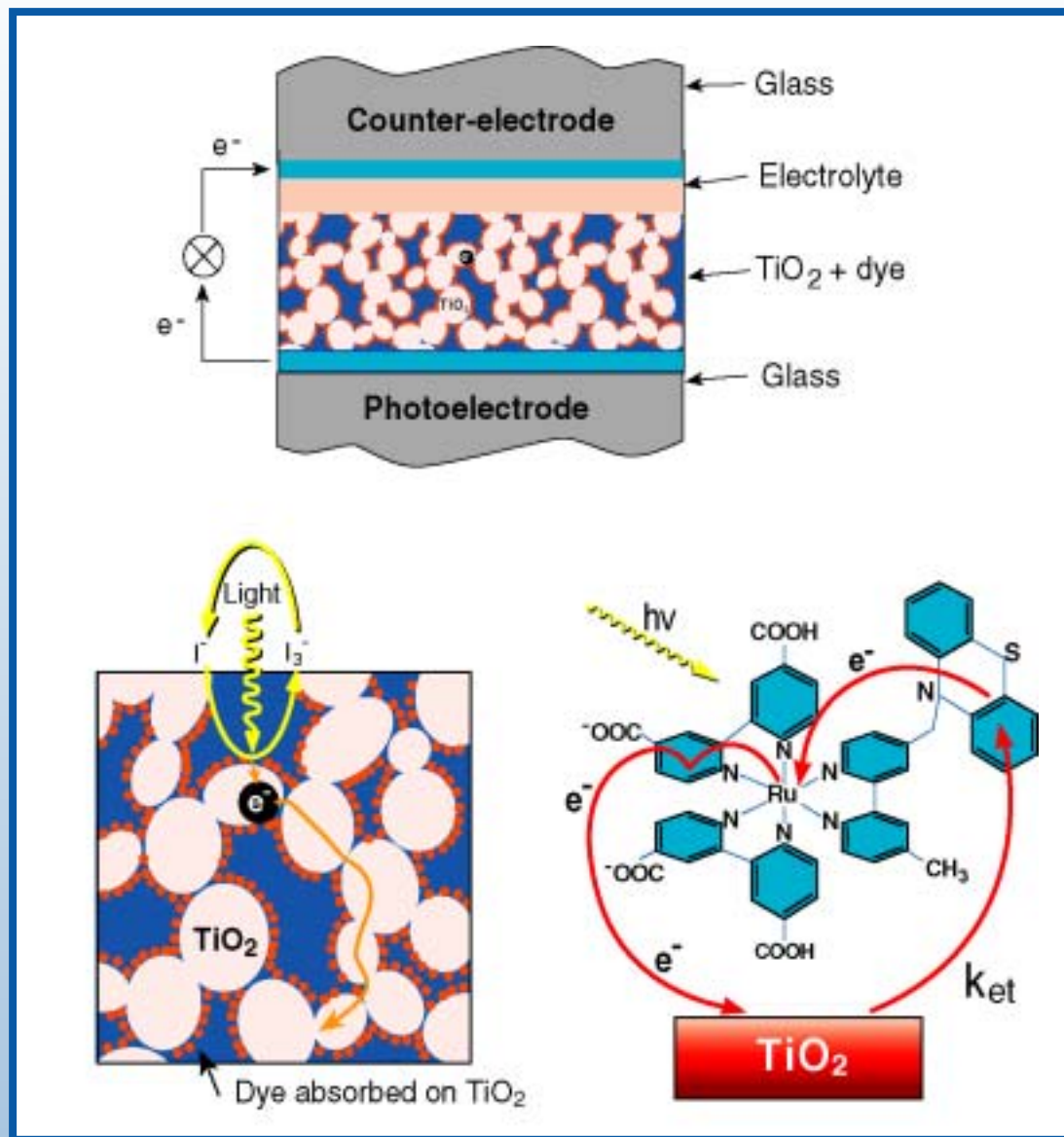
# Projects and Funding Sources



# Structure of 30.2%-efficient GaInP<sub>2</sub>/GaAs Two-Junction PV Cell



# Dye-Sensitized TiO<sub>2</sub> Solar Cell



03401631

# Valid Thermodynamic Approaches to Achieve Photon Conversion Efficiencies $> 32\%$ (Exceeding the Shockley-Queisser Limit)

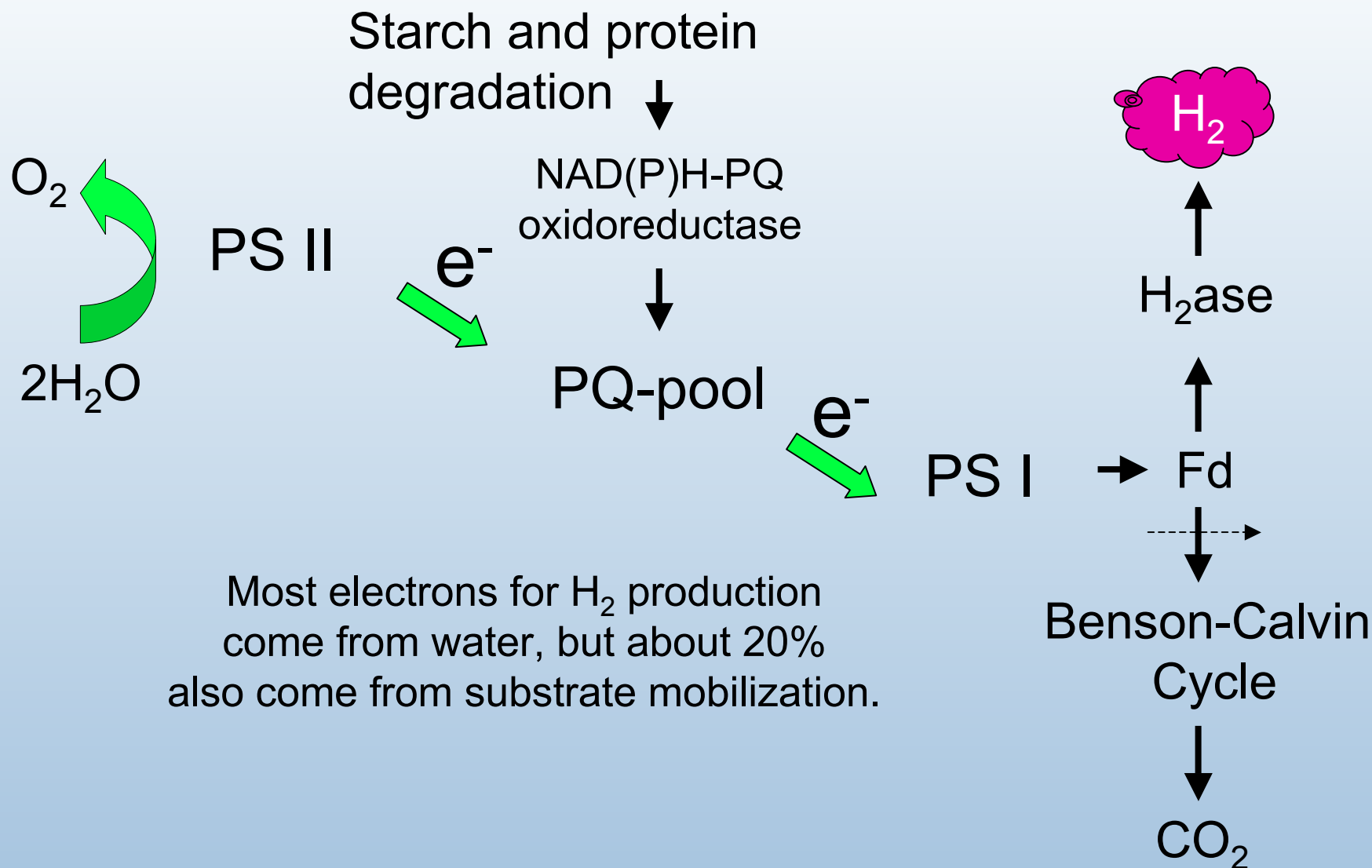
1. Tandem Cells
2. Hot Carrier Conversion
  - a. Extract, collect, and utilize hot carriers
  - b. Impact ionization
3. Intermediate Band Solar Cell
4. Thermophotonic Solar Cells
5. Down conversion and upconversion of incident photons

See:

M. Green, "Third Generation Photovoltaics". Springer, 2003

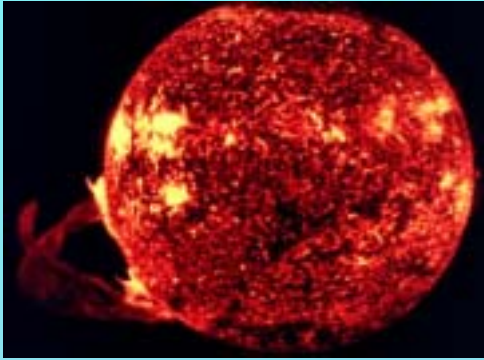
A. Marti and A. Luque, "Next Generation Photovoltaics", Inst. Of Physics Series in Optics and Optoelectronics, 2003

# Mechanism of H<sub>2</sub> Production



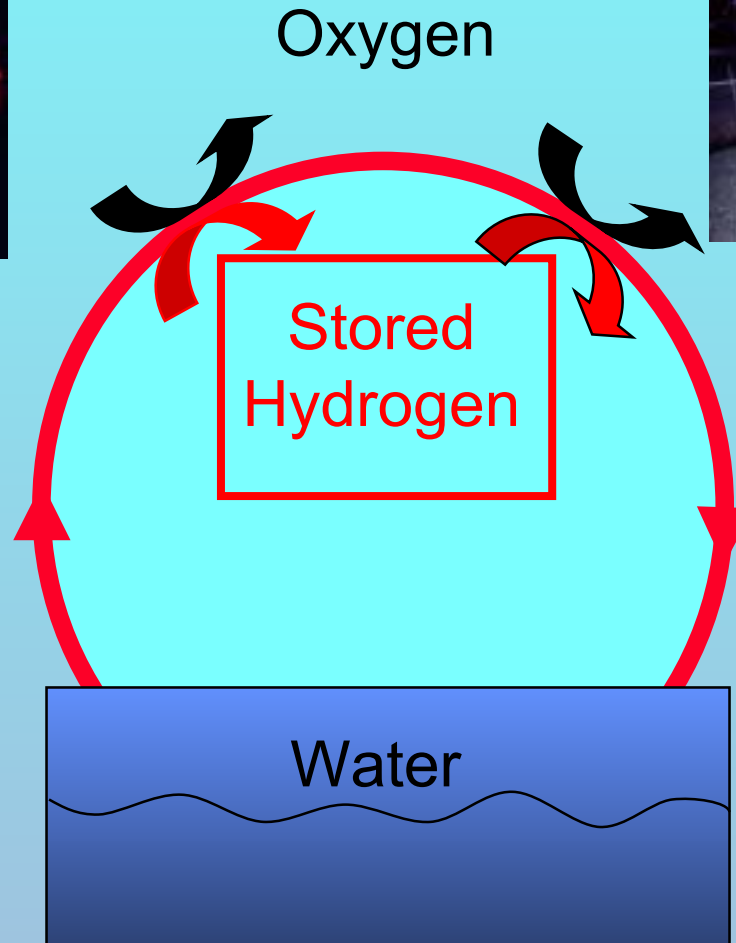


# Closed-Cycle Hydrogen Energy Economy



Inputs:

Solar Energy and  
Water



Outputs:

Electricity, heat  
and Water

# Summary of NREL's Activities in Nanoscience/Nanotechnology (concluded)

## Biotechnology

This research involves the integration of multi-subunit proteins, such as the bacterial cellulosomes, with nanoscience technologies in order to benefit from the self-assembly and modular nature of such proteins. NREL has worked in the fields of protein and metabolic engineering for nearly two decades. Much of the current focus, funded by DOE biofuels and industry, includes projects aimed at the improvement of cellulase enzymes by site-directed-mutagenesis and directed evolution, as well as the development of new microbial catalysts by manipulation of metabolic pathways. This work has resulted in 90 peer-reviewed publications, 4 books, and 12 patents.

## Applications

- Novel quantum dot arrays created with self-assembling proteins
  - Quantum dot solar lasers
  - Light-emitting diodes
  - Quantum dot photoconverters

# Why Employ the Electrodeposition Process

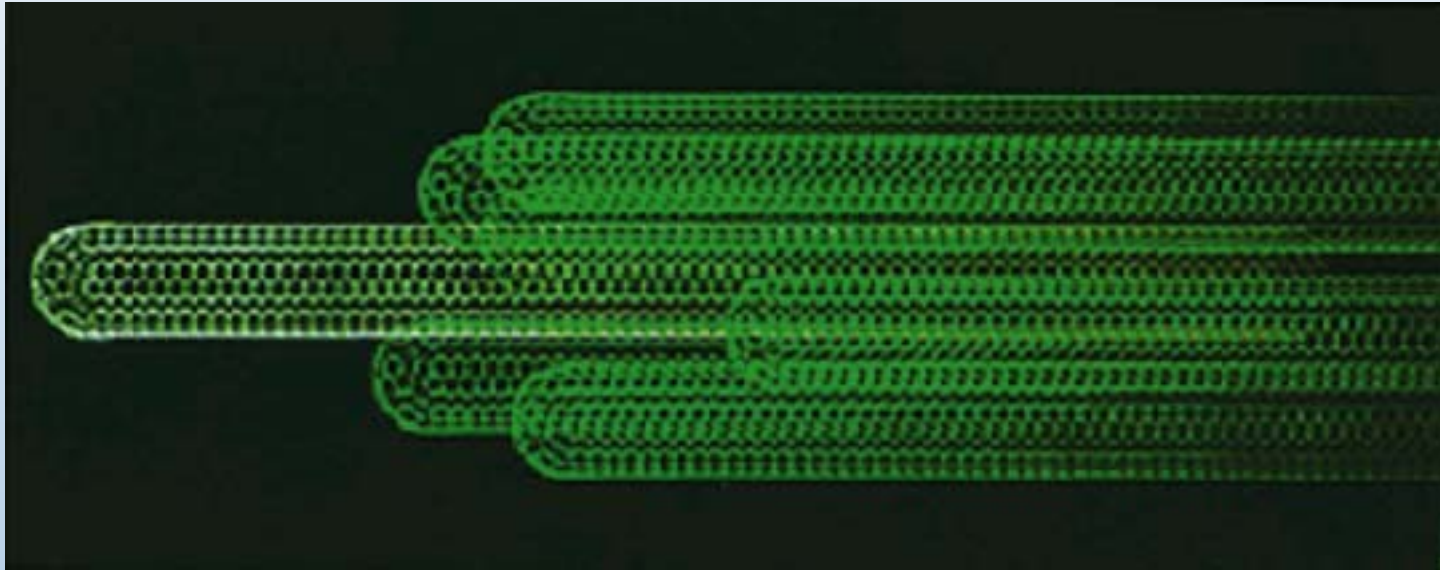
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# On-Board Hydrogen Storage Challenge

***Storing enough hydrogen on vehicles to achieve greater than 300 miles driving range is difficult.***

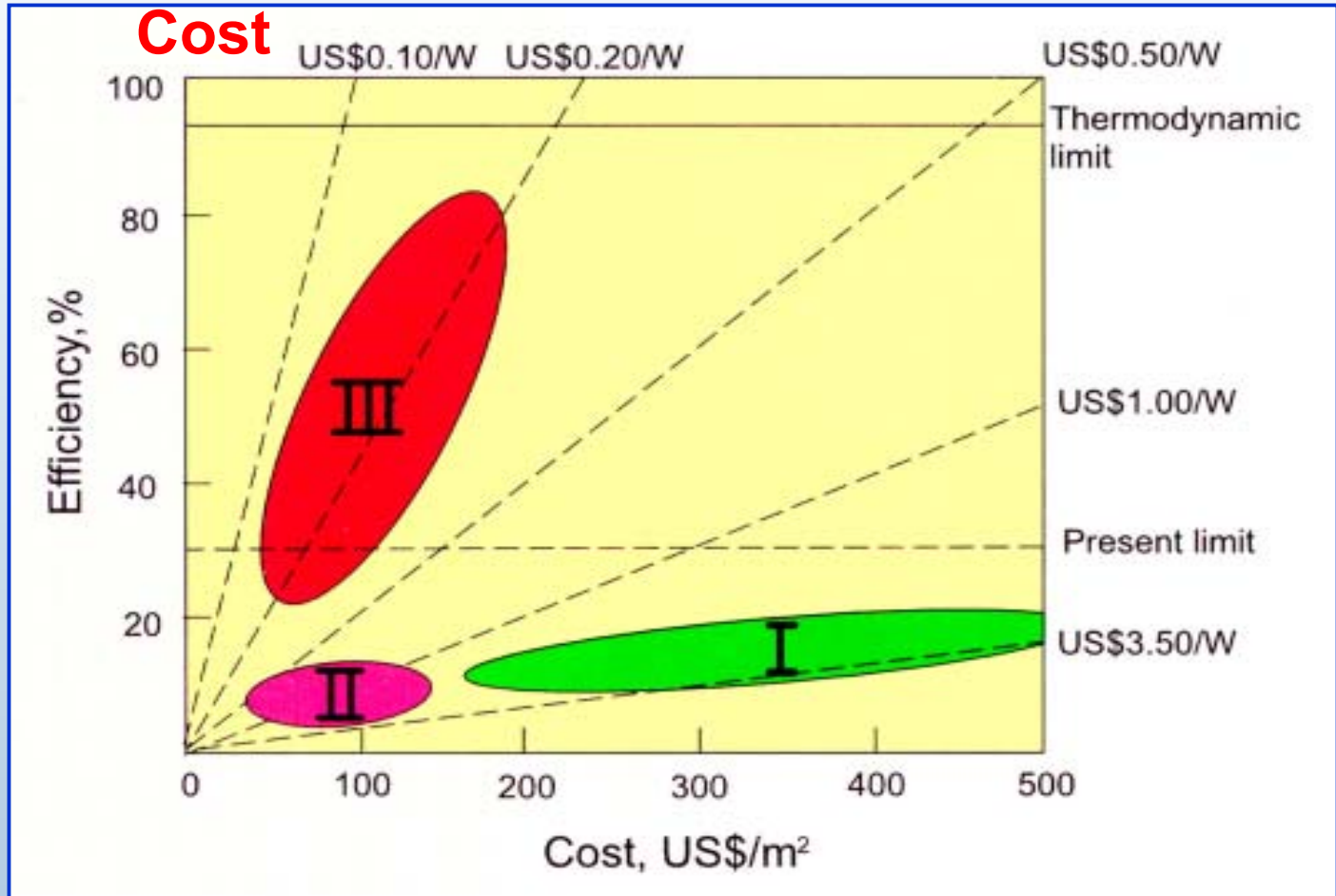
- On a weight basis  $H_2$  has nearly three times the energy content of gasoline.
  - 120 MJ/kg vs. 44 MJ/kg (LHV)
- On a volume basis the situation is reversed.
  - 3 MJ/L (5000 psi), 8 MJ/L ( $LH_2$ ) vs. 32 MJ/L
- Physical storage of hydrogen is bulky.
- Capacity of reversible chemical storage at useful T, P is low.
- Other challenging issues include energy efficiency, cost, and safety.

- Carbon Single-walled Nanotubes  
(SWNT)



# PV Power Costs as Function of Cell Efficiency and Module Cost

From:  
Martin Green,  
UNSW



For PV or PEC to provide the level of C-free energy required for electricity and fuel—power cost needs to be 2-3 cents/kWh (\$0.40 – \$0.60/W)